TRANSPORT PROBLEMS IN THE THEORY OF METALS

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A Thesis presented by

Neil Charles McGill

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Doctor of Philosophy.

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Declaration

I declare that this Thesis is my own composition, that it is based on research carried out by me, and that no part of it has previously been presented in application for a higher degree.

Certificate

I certify that in October 1965 Neil C. McGill was admitted as a Research Student under Ordinance General No.12 in the Department of Theoretical Physics of the University of St. Andrews; that he was admitted the following year as a candidate for the Degree of Doctor of Philosophy under Ordinance No. 16; that he has fulfilled the conditions of Ordinance No. 16 and the supplementary Senate regulations; and that he is qualified to submit the following Thesis in application for the Degree of Doctor of Philosophy.

Research Supervisor.

Career

In 1963 I graduated from the University of St. Andrews with a first class honours degree in Physics with Theoretical Physics. I then undertook a two year course of study and research in the Department of Materials of the College of Aeronautics, Cranfield (now the Cranfield Institute of Technology) and was awarded the Diploma of the College in 1965. In October that year I was admitted by the Senatus Academicus of the University of St. Andrews as a Research Student, and received financial support for one year from the Carnegie Trust for the Universities of Scotland. In 1966 I was appointed Assistant Lecturer in the Department of Theoretical Physics in the University of St. Andrews and was promoted to my present post as Lecturer in 1968.

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My overwhelming debt of gratitude is to my research supervisor Professor R.B. Dingle who suggested the problems tackled in this Thesis and without whose advice and encouragement the work would never have been finished. It is he who has made me realise that what seems at first to be impossible is sometimes not so.

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Finally I gratefully thank my wife for her unfailing moral support throughout and for the enthusiasm with which she has typed this Thesis.

CONTENTS

INTRODUCTION

Of all common substances, metals conduct heat and electricity to the greatest extent. They also exhibit very readily a range of more complicated phenomena - the galvanomagnetic, thermomagnetic and thermoelectric effects - which result when an electric field, a thermal gradient and a magnetic field are combined in various ways. Any theory of the metallic state, therefore, must explain why metals should demonstrate these properties as well as they do, and account for the variation of the physical quantities in question with temperature, electric field, atomic structure and so on.

It is now well established that the simplest metals are characterised by an energy band structure in which the topmost occupied band is half full, so making it easy to impart extra energy to those electrons lying at or just below the Fermi level. The electrons in this band are loosely bound to the atomic cores, and can readily move through the material. When an external electric field is applied, the average motion of such electrons in the direction of the field constitutes an electric current, while a thermal current results (in the presence of a thermal gradient) from the diffusion of electrons from hot to cold areas. Similar qualitative explanations may be furnished for the more complicated thermal, electric and magnetic effects.

Quantitatively, the key to the calculation of the transport coefficients - the electrical and thermal conductivities, the Hall coefficient, and so on - lies in the evaluation of the distribution function $f(\underline{r},\underline{k},t)$ which describes how the electrons are distributed in $(\underline{r},\underline{k})$ space at any time t. This function is found by solving the Boltzmann transport equation, the mathematical expression of the statement that any change in β with time is the sum of three contributions, one for each possible cause: diffusion, collisions, and the action of external fields. Even after simplifying assumptions have been made about the lattice through which the electrons move, the Boltzmann equation is, in its most general form, a complicated integral equation, the complexity stemming partly from the different types of electron collision which must all be represented: collisions with thermal vibrations of the lattice, with impurities, with other displaced atoms, with boundary surfaces, and so on. In practice relief is usually gained by considering only one or perhaps two of these types of collision at a time, assuming conditions which make these dominant. In the first problem to be considered here, attention is restricted mainly to the case where electrons are scattered by thermal vibrations of the lattice; in the second, the emphasis is on collisions which electrons make with the metal surface.

I.1. Scattering of Electrons by Thermal Vibrations.

Among the more complicated of the special cases of the Boltzmann equation (or Bloch equation, as it is often called in this context) is the one of probably greatest interest, i.e. where the electrons move through the crystal lattice with no hindrance save that provided by the thermal vibration of the ions. At temperatures higher than the Debye temperature, an approximate solution for β is relatively easily obtained, as will be demonstrated in Chapter 1.

For intermediate and low temperatures, attempts at finding a solution have included methods of successive approximation[1,2,17], a variational method[3] based on a minimum principle[5,6], and numerical evaluation[7]. These will be examined in Chapter 2; here it is relevant to point out that each, so far as it has yet been developed, has certain weaknesses and limitations. The number of successive approximations which can be evaluated is limited by the complexity of the mathematics, and no proper account of the convergence of the series can be given. The variational method does seem to yield values of the transport coefficients in tolerable agreement with experiment at both high and low temperatures; but it features the expansion of a function of unknown form as an infinite series of definite prescribed form, the coefficients being determined by the application of the minimum principle. Convergence of this series is once more unexaminable, nor is it certain that the true function is one for which a Taylor series representation exists. Numerical methods must of necessity assign numerical values to the parameters (such as temperature) which are involved, and no conclusive evidence of the analytic dependence of the interesting quantities on such parameters can emerge; in a sense, physical theory is thereby not advanced.

Thus no method so far suggested may be reckoned free from major deficiencies. There is scope for a new approach which will allow investigation of the mathematical properties of the functions which arise during the calculation, and so provide internal evidence for the validity of the entire method. Such an approach would also substantially assist further investigation of similar problems by the variational method. For in any application of the variational principle, it is obligatory to make some assumption about the form of the trial function to be used, and hitherto there has existed little evidence to support any particular assumption against possible alternatives. Even partial knowledge of the analytic properties of the functions which occur in this particular problem would go some way to guide and justify the choice of corresponding trial functions in this and similar problems, and hence fill a gap which still exists in this otherwise well-developed branch of physics.

A new method for solving the Bloch equation is presented in Part One of this thesis. Briefly, the procedure consists in expanding the unknown distribution function as an infinite double series in the two variables temperature and energy, and the discovery of a recurrence relation for the two-index coefficients. This recurrence relation is then examined, partly analytically and partly numerically, to elicit the dependence of the coefficient on the two indices. Though it has not been possible to achieve an exact solution of the recurrence equation, a sufficiently exact expression has been determined to permit the re-assembly of the double series to yield the required function. A fuller descriptive précis of this method is contained in the summary chapter at the beginning of Part One.

I.2. Scattering of Electrons by the Surfaces of a Thin Metal Film.

At all but very low temperatures, the "mean free path" for electrons, i.e. the mean distance travelled between collisions, is typically of the order of a few lattice spacings. This means that the influence of collisions with the metal surfaces is practically negligible for normal sized specimens, since the proportion of such collisions is extremely small. One is therefore justified in making the approximation $\partial f/\partial \underline{r} = 0$, and parameters such as the electrical conductivity are independent of the size and shape of the specimen.

This simple state of affairs breaks down under a suitable combination of (a) low temperature and (b) extreme smallness of the specimen in at least one direction. The electron mean free path is then of the same order as the thickness of the specimen, collisions with the surface must be explicitly analysed, and one cannot assume $\partial f / \partial \underline{r} = 0$. Depending on the extent to which electrons are specularly or diffusely reflected after collision, the tendency is for the resistivity of the specimen to be increased beyond that of the "bulk" metal.

To make progress with the Boltzmann equation when this extra complication arises, it is necessary to make simplifying assumptions about the <u>other</u> collision mechanisms which are operating. In particular, it is usual to postulate the existence of a "relaxation time" $\tau(\underline{k})$, i.e. in the absence of external fields, the function f always approaches its equilibrium value f_0 at a rate given by

$$\frac{\partial f}{\partial t} = - \frac{f - f_0}{\tau(\underline{k})}$$

It may be shown that this postulate is justified at high temperatures ($\gtrsim \theta_D$, the Debye temperature) and at very low temperatures when electron collisions are overwhelmingly due to impurities.
It is customary also to assume that electrons are quasi-free, i.e. $\underline{k} = m^* \underline{v}/\hbar$ where $\underline{v}$ is the velocity of an electron and m^* its effective mass. This means that $f(\underline{r}, \underline{k}, t)$ is equivalent to a function $N(\underline{r}, \underline{v}, t)$ which describes the distribution of electrons in $(\underline{r}, \underline{v})$ space at any time t.

With these assumptions it is possible to analyse the influence of metal surfaces on the electrical conductivity. For metal films and wires it has been shown by Fuchs[8] and by Dingle[9] respectively that the conductivity is a function of the thickness of the specimen divided by the mean free path. Comparison between theory and experiment can therefore yield information about the mean free path; unfortunately, however, such investigations are hampered by the need to use several specimens and the uncertainty in the knowledge of their exact respective thicknesses. [As pointed out by Chambers[11], it is in principle possible to base all measurements on a single specimen, but a dubious assumption is then required about the variation of the bulk conductivity with temperature.]

Partly in order to overcome such difficulties it is relevant to extend the theory to where there is a magnetic field present as well as an electric field. Under these new conditions, the trajectory of an electron between successive collisions is generally curved, and the conductivity depends on the momentum of the electrons as well as on the thickness of the film or wire. Comparison between theory and experiment is capable therefore of simultaneously yielding information about the momentum of the electrons at the Fermi surface and their mean free path. The conductivity increases with magnetic field (sometimes after an initial decrease) due to the modification to the trajectories of those electrons which in the absence of the field would have collided with the metal surface. To observe this - purely geometrical - effect, it is necessary that the normal bulk magnetoresistance should be as small as possible, i.e. that the conduction electrons should be nearly free. This limits reliable comparison of theory and experiment to group-1 metals.

Starting from a kinetic theory formulation[10] of transport phenomena, Chambers[11] has devised a graphical procedure for calculating the conductivity of thin <u>wires</u> in the presence of a longitudinal magnetic field, but no practical method of calculation appears to exist when the magnetic field is transverse. For thin <u>films</u>, there are three distinct orientations of the magnetic field with respect to the electric field. Solutions for the two transverse cases have been provided by Sondheimer[12] and by McDonald and Sarginson[13] and a comprehensive review of these and related work has been made by Sondheimer.[14]

The present work, which comprises Part Two of this thesis, is concerned with the remaining case where the fields are parallel. The solution depends on the two ratios d/r_0 and d/ℓ where d is the film thickness, r_0 the cyclotron radius and ℓ the bulk mean free path. An exact analytic solution valid for high fields only ($d \geqslant 2r_0$) has been found by Koenigsberg,[15] Azbel[16] and Barron and McDonald[21] while Kao[22] has computed the conductivity by direct numerical integration over a wide range of the magnetic field for a limited number of d/ℓ values.

Analysis of the solution for low and intermediate fields ($d < 2r_0$) leads, as will be shown, to various integrals which cannot be evaluated directly. The main purpose here is to devise analytic methods for expressing these approximately in terms of known functions. This approach, in contrast to resorting to direct numerical integration for this particular problem only, represents a first step in the selection and development of the best approximations to the many more complicated problems in this class. The approximations foundprovide a convenient way of evaluating the conductivity to adequate accuracy for all but a limited range of the parameters. The validity of the results obtained has been confirmed by comparing them with those of Kao; experimental evidence for the effect is also discussed.

The work presented in Part Two has already been published[20] in substantially similar form. A concise summary of the methods employed is displayed in the summary chapter at the beginning of Part Two.

Part One

A NEW METHOD OF SOLUTION TO THE BLOCH INTEGRAL EQUATION IN THE THEORY OF METALS

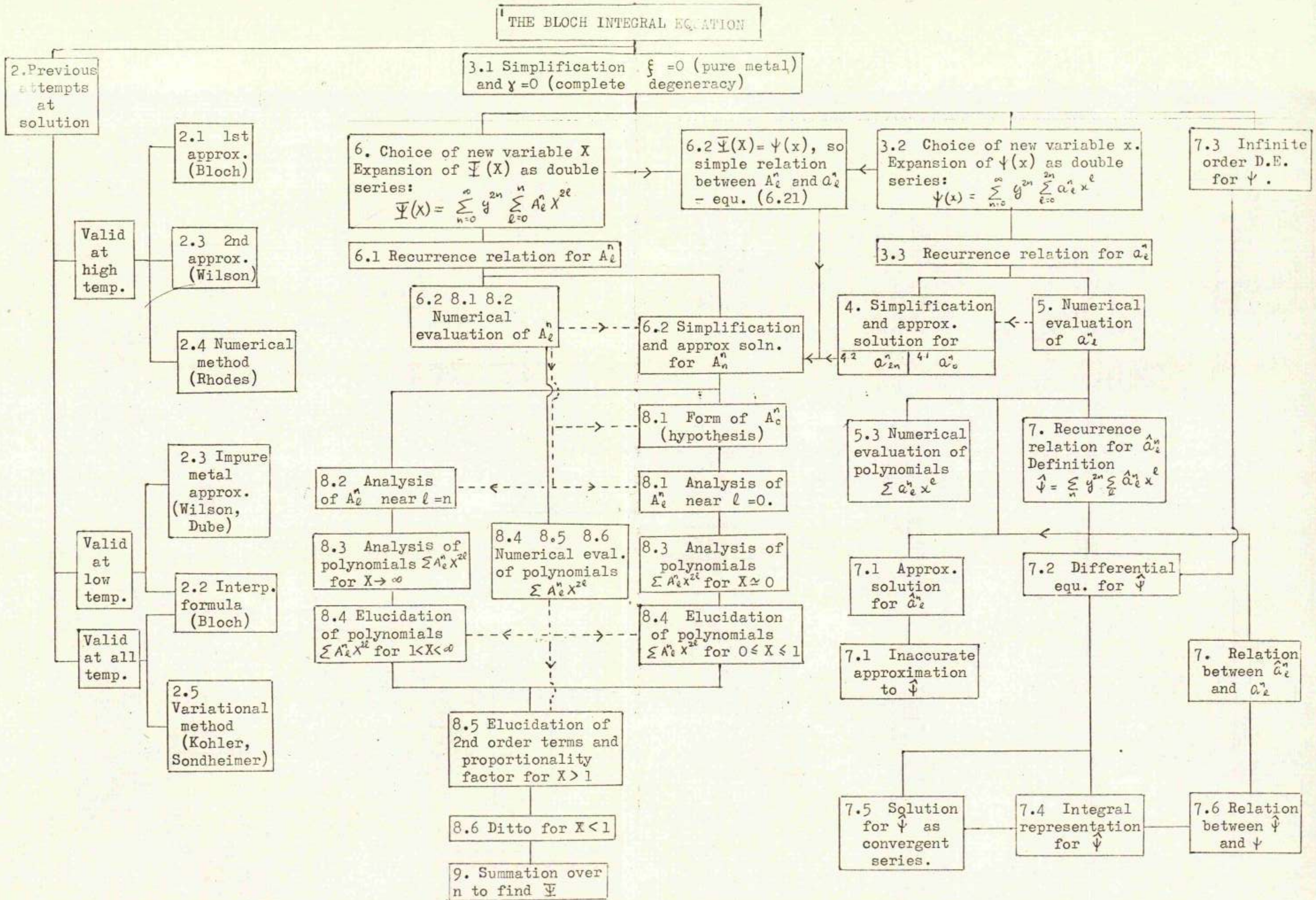
SUMMARY OF PART ONE

The development of the argument in Part One is of necessity somewhat labyrinthine, and it is convenient to display the connection between the various constituents on the attached chart. The general flow of the argument is from top to bottom, arrows indicating the direction where there is possible ambiguity. The numbers in the boxes refer to chapters and sections of chapters in Part One. Dotted lines indicate where computer calculations have served as a check on either (a) existing analytically-derived relations or (b) hypotheses, e.g. concerning the form of variation of coefficients with their indices. Arrows show the direction of flow of information provided by such calculations.

With the aid of the chart, the complete argument may be summarised chapter by chapter as follows:

Chapter 1 In this opening chapter the Bloch equation is set up and cast into the most suitable form for subsequent analysis.

The chapter begins with a brief derivation of Boltzmann's equation (§ 1.1) without explicit calculation of $(\partial f/\partial t)_{collisions}$. General expressions for this quantity are quoted without proof in § 1.2 for (a) collisions with phonons and (b) collisions with impurities. With their aid, the Bloch integral equation then follows. It is shown that a time of relaxation exists at high temperatures only. For arbitrary temperatures (§ 1.3) the distribution function is re-expressed in terms of the two "formal relaxation times" defined by Dingle[19], whereupon the original integral equation splits into two


THE BLOCH INTEGRAL EQUATION
2. Previous attempts at solution
3.1 Simplification ξ = 0 (pure metal) and γ = 0 (complete degeneracy)
2.1 1st approx. (Bloch)
Valid at high temp.
2.3 2nd approx. (Wilson)
2.4 Numerical method (Rhodes)
2.3 Impure metal approx. (Wilson, Dube)
Valid at low temp.
2.2 Interp. formula (Bloch)
Valid at all temp.
2.5 Variational method (Kohler, Sondheimer)
6. Choice of new variable X Expansion of $\Psi(X)$ as double series: $\Psi(X) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{n} A_\ell^n X^{2\ell}$
6.2 $\Psi(X) = \psi(x)$, so simple relation between A_ℓ^n and a_ℓ^n – equ. (6.21)
3.2 Choice of new variable x. Expansion of $\psi(x)$ as double series: $\psi(x) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n} a_\ell^n x^\ell$
7.3 Infinite order D.E. for ψ.
6.1 Recurrence relation for A_ℓ^n
3.3 Recurrence relation for a_ℓ^n
6.2 8.1 8.2 Numerical evaluation of A_ℓ^n
6.2 Simplification and approx soln. for A_n^n
4. Simplification and approx. solution for
4.2 a_{2n}^n
4.1 a_0^n
5. Numerical evaluation of a_ℓ^n
8.1 Form of A_0^n (hypothesis)
5.3 Numerical evaluation of polynomials $\sum a_\ell^n x^\ell$
7. Recurrence relation for $\hat{a}_\ell^n$ Definition $\hat{\psi} = \sum_n y^{2n} \sum_\ell \hat{a}_\ell^n x^\ell$
8.2 Analysis of A_ℓ^n near $\ell = n$
8.1 Analysis of A_ℓ^n near $\ell = 0$.
8.3 Analysis of polynomials $\sum A_\ell^n X^{2\ell}$ for $X \to \infty$
8.4 8.5 8.6 Numerical eval. of polynomials $\sum A_\ell^n X^{2\ell}$
8.3 Analysis of polynomials $\sum A_\ell^n X^{2\ell}$ for $X \simeq 0$
7.1 Approx. solution for $\hat{a}_\ell^n$
7.2 Differential equ. for $\hat{\psi}$
8.4 Elucidation of polynomials $\sum A_\ell^n X^{2\ell}$ for $1 < X < \infty$
8.4 Elucidation of polynomials $\sum A_\ell^n X^{2\ell}$ for $0 \leq X \leq 1$
7.1 Inaccurate approximation to $\hat{\psi}$
7. Relation between $\hat{a}_\ell^n$ and a_ℓ^n
8.5 Elucidation of 2nd order terms and proportionality factor for $X > 1$
8.6 Ditto for $X < 1$
9. Summation over n to find Ψ
7.5 Solution for $\hat{\psi}$ as convergent series.
7.4 Integral representation for $\hat{\psi}$
7.6 Relation between $\hat{\psi}$ and ψ

separate integral equations for the two relaxation times. Finally, these are cast into a non-dimensional form similar to that adopted by Rhodes[7]. Mathematically, the problem is to solve the two integral equations for the two unknown functions $\phi(\eta)$ and $\phi^*(\eta)$. [$\eta = (E-\zeta)/kT$ where E is the electron energy, ζ the Fermi potential, k Boltzmann's constant and T the absolute temperature.]

Chapter 2 Here a review is made of previously derived approximate solutions of the Bloch equation, in roughly historical order.

The elementary first order high-temperature approximation due to Bloch[17] is described in § 2.1. The same author[1] elucidated the first order term in a low temperature series for the distribution function, which contrives to duplicate the known behaviour in the high temperature limit. It therefore possesses the status of an interpolation formula valid at all temperatures (§ 2.2).

The second-order terms for a pure metal at high temperatures have been elucidated by a method of successive approximations invented by Wilson[2]. (A previous attempt by Brillouin[42] to find these terms has been proved invalid - the reasons for this are discussed.). A similar calculation of the second order terms for an impure metal at low temperatures appeared in the same paper; this work was soon extended by Dube[41].

§ 2.4 comprises a description of the numerical method devised by Rhodes[7] for extending the range of validity of the high-temperature solution. An improved first-order approximation is found, and the method of successive approximations then applied numerically for the solution of the integral equation.

The final section § 2.5 states the variational principle found by Kohler[5,6] as a condition on the required solution; this has been employed both by Kohler and by Sondheimer[3] to find the coefficients in a trial expansion of the unknown distribution function when the latter is substituted into the integral equation.

<u>Chapter 3</u> In § 3.1 it is assumed that there is no impurity scattering and that the electron gas is completely degenerate. ($\gamma = kT/\zeta$ may be taken to be zero.) The two integral equations for ϕ and ϕ^* then become identical, so that $\phi^* = \phi$ in this approximation.

A new variable $x = (1+e^{\eta})^{-1}$ is selected (§ 3.2) and $\phi(\eta) \equiv \psi(x)$ can now be expanded in the form

$$\psi(x) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n} a_\ell^n x^\ell \tag{S.1}$$

where $y = \theta_D/T$, θ_D being the Debye temperature. Substituting in the integral equation, a recurrence relation for the coefficient a_ℓ^n is found by equating equal powers of y and x on the two sides of the equation (§ 3.3).

<u>Chapter 4</u> The general recurrence relation for a_ℓ^n is quite complicated, but becomes much simpler in form at the two extremities in the range of ℓ - values, viz. $\ell = 0$ and $\ell = 2n$. An approximate solution for a_0^n, valid when n is large, can be found relatively easily (§ 4.1) and a similar but more complicated argument yields a corresponding solution for a_{2n}^n (§ 4.2).

<u>Chapter 5</u> The coefficients a_ℓ^n and polynomials $\sum a_\ell^n x^\ell$ have been evaluated numerically by digital computer, in the latter case for various values of x, with the following aims and results:

(i) Confirmation of the expressions for a_0^n and a_{2n}^n derived analytically in the previous chapter, and improvement of the accuracy of any approximate parameters involved.

(ii) Inspection of the variation of a_ℓ^n with n and ℓ. It is found that a_ℓ^n generally rises in value quite rapidly with n, and reaches a peak with variation in ℓ at about $\ell = \frac{3}{2}n$ In particular it is observed that, of the various contributions to a_ℓ^n in the recurrence relation, those involving a_s^{n-1} $(s = 0, 1 \ldots, 2n-2)$ are dominant. This is made the basis of an approximation to a_ℓ^n , denoted by $\hat{a}_\ell^n$,which is introduced and discussed in Chapter 7. Also, the ratio of a_ℓ^n to a_{2n}^n is, to a good approximation, $(-1)^\ell$ times the binomial coefficient $\binom{\ell}{2n-\ell}$. This is exploited in § 7.1 to yield an approximate solution for $\hat{a}_\ell^n$.

(iii) Inspection of the values of the polynomials $\sum a_\ell^n x^\ell$. These are observed to be much smaller, numerically, than the coefficients a_ℓ^n themselves; despite this, they gradually increase in magnitude approximately as $(2n)!$, (except when $x = 0$), indicating that the series over n in (S.1) is asymptotic. The limited utility of this series for direct numerical estimation of ψ is noted.

Chapter 6 The choice of the variable x in Chapter 3 is, unfortunately, not completely satisfactory, since $\psi(x) = \psi(1-x)$ and the coefficients a_ℓ^n are therefore not all independent. The coefficients are also much bigger than the polynomials to which they contribute, so the process of calculating the latter is computationally inefficient. Finally $x = 0$ is an atypical point in the range $0 \leq x \leq 1$ for the behaviour of the polynomials $\sum a_\ell^n x^\ell$.

A new variable $X = 1-2x$ has therefore been chosen and the function $\Psi(X)$ $[= \psi(x)]$ expanded in the form

$$\Psi(X) = \sum_{n=0}^{\infty} g^{2n} \sum_{\ell=0}^{n} A_\ell^n X^{2\ell}. \tag{S.2}$$

The recurrence relation for A_ℓ^n is found (§ 6.1) from the original integral equation by a process similar to that for a_ℓ^n described in Chapter 3. From this, the coefficients A_ℓ^n and polynomials $\sum A_\ell^n X^{2\ell}$ may be calculated by digital computer (§ 6.2). The former turn out to be much smaller in magnitude than the coefficients a_ℓ^n (for given n) and are of course all independent. The variation with n of the polynomials $\sum A_\ell^n X^{2\ell}$ at $X = 0$ is entirely typical.

Although the recurrence relation for A_ℓ^n is even more complicated than that for a_ℓ^n, it simplifies greatly at $\ell = n$ to permit an approximate solution for large n. This solution can also be deduced as a particular case of the general relation connecting the A_ℓ^n and a_ℓ^n coefficients, resulting from the equality of $\psi(x)$ and $\Psi(X)$. When $\ell = n$, the relation reduces to

$$A_n^n = a_{2n}^n \left(\tfrac{1}{2}\right)^{2n}, \tag{S.3}$$

the coefficient a_{2n}^n having already been elucidated in §4.2.

<u>Chapter 7</u> The observation in Chapter 5 that, numerically, the coefficients a_ℓ^n are determined mainly by those contributions in the recurrence relation involving the a_s^{n-1} $(s = 0, 1, \ldots 2n-2)$, prompts the definition of a new set of coefficients $\hat{a}_\ell^n$ through a modified recurrence relation which retains only the most important contributions. One would expect that $\hat{a}_\ell^n$ would be an approximation in some sense to a_ℓ^n and that the corresponding function

$$\hat{\psi}(x) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell \tag{S.4}$$

would be related to the required function ψ. Numerically, the coefficients $\hat{a}_\ell^n$ match the behaviour of a_ℓ^n with variation in n and ℓ but are smaller in magnitude.

It is shown in §7.1 that a reasonably good empirical solution for $\hat{a}_\ell^n$, inspired by the observations made in Chapter 5 and valid near $\ell = n$, is nevertheless incapable of yielding a good approximation to $\hat{\psi}$. The best way to find $\hat{\psi}$ is first to construct the second order differential equation for $\hat{\psi}$ from the recurrence relation for $\hat{a}_\ell^n$ (§7.2) and then solve it. (Alternatively, this differential equation can be obtained by retaining the most significant terms in an infinite order differential equation for

ψ (§ 7.3) derived from the original integral equation.) The required solution $\hat{\psi}$ may be represented in two different but equivalent forms - as an integral representation (§ 7.4) or as a converging series (§ 7.5). Finally the relation between $\hat{\psi}$ and ψ is considered in § 7.6.

Chapter 8 The observation that the variation with n of the polynomials $\sum A_\ell^n X^{2\ell}$ at X = 0 is fairly typical of that for X $\simeq$ 0 makes it desirable to elucidate the approximate dependence of A_ℓ^n on n and ℓ near ℓ = 0, since these are the coefficients which contribute most to the polynomial. § 8.1 consists therefore of an analysis of the form of A_0^n followed by a similar investigation of A_ℓ^n for small $\ell \neq$ 0. At each stage a hypothesis is made, based on the analytic and numerical information so far elicited, which is tested numerically by insertion of the appropriate values of A_ℓ^n.

In § 8.2 a similar procedure is reported for the coefficients A_ℓ^n in the neighbourhood of ℓ = n. (The form of A_n^n itself is already known from § 6.2, which simplifies the analysis compared with the region $\ell \simeq$ 0.) The reason for requiring this information is that the highest order coefficients A_n^n, A_{n-1}^n, etc. dominate the form of the polynomial as X $\to \infty$. Although the region of X of physical interest is 0 $\leq$ X $\leq$ 1, it is instructive also to calculate the polynomials for values of X in the 'non-physical' region 1 $<$ X $< \infty$, since knowledge of their behaviour in this region is more easily elucidated and provides a valuable guide to the expected behaviour in the 'physical' region.

By this stage there is sufficient information to calculate the approximate form of the polynomials in the two regions X $\simeq$ 0 and X $\to \infty$. (§ 8.3). A reasonable deduction can then be made of the probable form of the polynomials in the two regions 0 $\leq$ X $\leq$ 1 and 1 $<$ X $< \infty$, the two hypotheses concerned being checked by numerical analysis (§8.4). The analytic forms of the two functions concerned are found by further numerically - verified hypotheses. In §8.5 the accuracy of the expression for $X > 1$ is improved by investigating the second order term and the proportionality factor, at first numerically and then analytically. Finally, in §8.6, the corresponding factors for $X < 1$ are found by requiring the expression for $X > 1$ to carry over to that for $X < 1$ when we analytically continue all functions from one region to another.

Chapter 9 Now that the approximate analytic form of the polynomials $\sum A^n_\ell X^{2\ell}$ is known, the way is clear to calculate the function Ψ by summing over n in (S.2). Two procedures are distinguished, one appropriate at moderate and high temperatures (§9.1), the other at low temperatures (§9.2). In the first, the decreasing terms of the asymptotic series are retained exactly, the others being approximated by our formula for late terms. The sum of late terms is interpreted via Dingle's 'converging factors'[48], and the resulting expression for Ψ is demonstrated to be capable of yielding accurate results over the temperature range considered.

At low temperatures, successive terms increase from the outset and it is preferable to sum over n from 1 to ∞. It is then necessary to include a series contribution to Ψ arising from the difference between the actual coefficients of y^{2n} in (S.2) and the expression which approximates late polynomial behaviour. It is shown that this 'residual series' must be the most dominant component of Ψ at very low temperatures, since then the other summed contributions are certainly of minor importance. For the particular case $X = 0$, support for this conclusion is demonstrated by direct numerical estimation of this 'residue' and of its variation with temperature.

Chapter 10 Here a summary is briefly made of the main procedures devised and conclusions drawn to date. A few suggestions are made as to how the solution obtained for Ψ might be improved and generalised. The principles involved in the application of the new method to the problem of polar semiconductors are briefly discussed, and the extremely interesting first results of such an analysis are reported.

Chapter 1.

DERIVATION OF THE BLOCH INTEGRAL EQUATION

In this chapter the Bloch integral equation is set up and cast into the most suitable form for subsequent analysis.

1.1 The Boltzmann Equation

An electron moving through a perfectly periodic crystal lattice has a wave function of the form

$$\psi_{\underline{k}}(\underline{r}) = e^{i\underline{k}\cdot\underline{r}}\, u_{\underline{k}}(\underline{r}) \tag{1.1}$$

where $\underline{k}$ denotes the state of the electron, $\underline{r}$ its position and the function $u_{\underline{k}}(\underline{r})$ is periodic in the lattice. It was first shown by Bloch[17] that such electrons give rise to an unchanging current, so that non-zero values of electrical resistivity must be attributed to deviations from perfect periodicity. The latter is most commonly due to (a) defects of the crystal - impurity atoms, vacant sites, dislocations etc. - and (b) thermal vibrations of the lattice (phonons) which displace each atom in turn from its equilibrium position. Thus calculation of the electric and thermal conductivities and the other physical quantities of interest depends crucially on knowledge of the extent to which electrons are scattered by lattice imperfections.

At time t, let the number of electrons whose combined $(\underline{r}, \underline{k})$ vector lies in the "volume" element $d^3\underline{r}\; d^3\underline{k}$ be

$$\frac{1}{4\pi^3}\, f(\underline{k}, \underline{r}, t)\, d^3\underline{r}\; d^3\underline{k} \quad . \tag{1.2}$$

The function f varies with time due to (i) diffusion,

(ii) acceleration caused by external fields, and (iii) collisions, so that

$$\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{diff.} + \left(\frac{\partial f}{\partial t}\right)_{fields} + \left(\frac{\partial f}{\partial t}\right)_{coll.} \quad . \tag{1.3}$$

With the aid of Liouville's theorem

$$\frac{d}{dt}\left(d^3\underline{r}\ d^3\underline{k}\right) = 0 \quad , \tag{1.4}$$

a straightforward calculation shows that

$$\left(\frac{\partial f}{\partial t}\right)_{diff.} = -\underline{v}_{\underline{k}} \cdot \frac{\partial f}{\partial \underline{r}} \quad , \tag{1.5}$$

$$\left(\frac{\partial f}{\partial t}\right)_{fields} = \frac{e}{\hbar}\left(\underline{\mathcal{E}} + \frac{1}{c}\,\underline{v}_{\underline{k}} \times \underline{H}\right) \cdot \frac{\partial f}{\partial \underline{k}} \quad . \tag{1.6}$$

Here $(-e)$ is the electronic charge, $\underline{\mathcal{E}}$ and $\underline{H}$ are the applied electric and magnetic fields, and $\underline{v}_{\underline{k}}$ is the velocity of an electron in state $\underline{k}$. Combining (1.3), (1.5) and (1.6), we have Boltzmann's equation

$$\frac{\partial f}{\partial t} + \underline{v}_{\underline{k}} \cdot \frac{\partial f}{\partial \underline{r}} - \frac{e}{\hbar}\left(\underline{\mathcal{E}} + \frac{1}{c}\,\underline{v}_{\underline{k}} \times \underline{H}\right) \cdot \frac{\partial f}{\partial \underline{k}} = \left(\frac{\partial f}{\partial t}\right)_{coll.} \tag{1.7}$$

on whose solution depends the whole range of electrical, thermal and magnetic properties which derive from the transport of electrons through the lattice.

It is well known that the distribution function f for electrons in thermodynamic equilibrium is the Fermi-Dirac function

$$f_0(\underline{k}) = \left[\exp\left(E_{\underline{k}} - \zeta\right)/kT + 1\right]^{-1} \tag{1.8}$$

where $E_{\underline{k}}$ is the energy of an electron in state $\underline{k}$, ζ is the Fermi potential, k is Boltzmann's constant and T is the absolute temperature. The value of ζ is determined by the number of electrons per unit volume:

$$n = \frac{1}{4\pi^3} \int \frac{d^3k}{\exp(E_k - \zeta)/kT + 1} \tag{1.9}$$

When the temperature varies with $\underline{r}$ but no net transport of electrons occurs, we assume that there still exists an equilibrium function $f_0(\underline{k}, \underline{r})$ given by the R.H.S. of (1.8) where T and ζ are now functions of $\underline{r}$.

When $\underline{E}$ and $\underline{H}$ are zero and f is not a function of position, $\partial f/\partial t$ is just $(\partial f/\partial t)_{coll.}$ by(1.7). Under these circumstances it is plausible, though not necessary, that $\partial f/\partial t$ - the rate at which f returns to its equilibrium value - should be proportional to the difference between f and the equilibrium function f_0, i.e.

$$\left(\frac{\partial f}{\partial t}\right)_{coll.} = - \frac{f - f_0}{\tau(\underline{k})} \tag{1.10}$$

where $\tau(\underline{k})$ is a characteristic "relaxation time", whose functional form may be assumed to vary with the scattering mechanism operating.

When a relaxation time exists, the solution of the Boltzmann equation is considerably simplified and explicit expressions for the electrical and thermal conductivities and the other quantities of interest are easily derived,[18] even though additional assumptions and approximations may be required for their numerical evaluation. However the premise that a relaxation time exists is by no means generally valid: where, for example, the electron scattering is caused by thermal vibration of the lattice, it turns out to be legitimate at high temperatures only, as will be shortly demonstrated.

1.2. The Calculation of $(\partial f/\partial t)_{coll.}$

In the case of scattering due to lattice vibrations, the calculation of $(\partial f/\partial t)_{coll.}$ is rather long and complicated and expositions of the theory are readily obtainable.[18] For these reasons it will be convenient simply to state the result, after an enumeration of the (sometimes rather drastic) assumptions which must be introduced at various stages in the argument to make it mathematically tractable. These are:

(i) The crystal lattice is Bravais.

(ii) We may neglect terms higher than quadratic in the expansion of the total potential energy of the lattice as a series in rising powers of the displacement of the ions from their equilibrium positions.

(iii) Lattice vibrations are approximately independent of the motion of the electrons, coupling between them occurring only through the change in electron potential energy caused by displacement of the ions.

(iv) We may neglect the so-called Umklapp processes, those in which momentum is imparted to the crystal as a whole during a phonon-electron interaction.

(v) The potential for an electron inside a given unit cell is dominated by the contribution from the ion which occupies it.

(vi) The function $u_{\underline{k}}(\underline{r})$ - the periodic part of the Bloch wave function (1.1) for an electron moving through a perfect lattice (no phonons) - does not vary much with $\underline{k}$, is spherically symmetrical inside the atomic core and almost constant outside it.

(vii) $E_{\underline{k}} = \hbar^2 |\underline{k}|^2 / (2m^*)$ where m^* is the electron effective mass.

(viii) The phonon spectrum is the equilibrium one, characterised by the Bose-Einstein distribution function $[e^{h\nu/kT} - 1]^{-1}$, ν being the phonon frequency.

(ix) The velocity of sound does not vary with wavelength.

(x) There exist only an electric field and a temperature gradient both aligned in the x-direction, and squares of these quantities may be neglected.

(xi) The number of free electrons is $\gtrsim \frac{1}{4}$ (number of atoms). (This is the assumption which specifies that we are dealing with metals. The other case ($\lesssim$ instead of $\gtrsim$) leads us to the corresponding theory for semiconductors, which does not pose nearly the same problems as for metals, and will not be discussed further).

With all these assumptions and approximations, $(\partial f/\partial t)_{coll.}$ is

$$\left(\frac{\partial f}{\partial t}\right)_{coll.} = k_x \frac{\partial f_0}{\partial E} \frac{\sqrt{m^*/2}}{\hbar^2 \Lambda E^{3/2}} \left(\frac{T}{\Theta_D}\right)^3 \int_{-\Theta_D/T}^{\Theta_D/T} \left\{ E\, C(\eta) - C(\eta+z)\left[E + \tfrac{1}{2}kTz - D\left(\frac{T}{\Theta_D}\right)^2 z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|} . \tag{1.11}$$

Here k_x is the x component of $\underline{k}$, Θ_D is the Debye temperature, $\eta = (E - \zeta)/kT$, $z = h\nu/kT$ and $C(\eta)$ is defined by

$$f(\underline{k}) = f_0(\underline{k}) - k_x \frac{\partial f_0}{\partial E} C(\eta) . \tag{1.12}$$

In addition,

$$\Lambda = \left(\frac{4\pi}{3}\right)^{1/3} \frac{4 M a k \Theta_D}{3 h^2 C^2} , \tag{1.13}$$

$$D = \frac{(6\pi^2)^{2/3} \hbar^2}{4 m^* a^2} , \tag{1.14}$$

where M is the ionic mass, a^3 is the volume of a unit cell, and C is an integral over the unit cell involving the function $u_{\underline{k}}(\underline{r})$ whose value is taken to be approximately constant.

When scattering is due to lattice impurities, the corresponding calculation of $(\partial f/\partial t)_{coll.}$ is considerably simpler. With the assumptions (vii) and (x) above it can be shown[18] that

$$\left(\frac{\partial f}{\partial t}\right)_{coll.} = k_x \frac{\partial f_0}{\partial E}\sqrt{\frac{2}{m^*}}\ \frac{E^{1/2}}{\ell}\ c(\eta) \tag{1.15}$$

where ℓ is the mean free path between collisions.

When both scattering mechanisms exist, the total value of $(\partial f/\partial t)_{coll.}$ is the sum of (1.11) and (1.15). Now assumptions (vii) and (x) simplify the Boltzmann equation to

$$-\frac{\hbar}{m^*} k_x \frac{\partial f_0}{\partial E}\left[e\mathcal{E} + T\frac{\partial}{\partial x}\left(\frac{\zeta}{T}\right) + \frac{E}{T}\frac{\partial T}{\partial x}\right] = \left(\frac{\partial f}{\partial t}\right)_{coll.} . \tag{1.16}$$

Hence, combining (1.11), (1.15) and (1.16), we have

$$e\mathcal{E} + T\frac{\partial}{\partial x}\left(\frac{\zeta}{T}\right) + \frac{E}{T}\frac{\partial T}{\partial x} = -\frac{\sqrt{2m^*}}{\hbar}\frac{E^{1/2}}{\ell}c(\eta)$$

$$-\frac{m^{*3/2}}{\sqrt{2}\hbar^3\Lambda E^{3/2}}\left(\frac{T}{\Theta_D}\right)^3\int_{-\Theta_D/T}^{\Theta_D/T}\left\{E\,c(\eta) - c(\eta+z)\left[E + \tfrac{1}{2}kTz - D\left(\frac{T}{\Theta_D}\right)^2 z^2\right]\right\}\frac{e^{\eta}+1}{e^{\eta+z}+1}\ \frac{z^2\,dz}{|1-e^{-z}|}$$

$$(1.17)$$

which is an inhomogeneous integral equation for the unknown function $c(\eta)$. This equation is sometimes referred to as the Bloch equation after F. Bloch who first derived and discussed it.[17]

It is now easy to see that a time of relaxation exists only at high temperatures. From the definitions (1.10) and (1.12), the existence condition is that $(\partial f/\partial t)_{coll.}$ should be proportional to $c(\eta)$. This condition is already satisfied for the lattice impurity contribution (1.15) and is also satisfied for phonon scattering in the limit $\Theta_D/T \rightarrow 0$, when only the first term is significant in an expansion of the integrand in (1.11) in rising powers of z. (This corresponds to the reduction of (1.17) to an ordinary equation for $c(\eta)$). In this limit, the reciprocal of the total relaxation time is the sum of two contributions:

$$\frac{1}{\tau(E)} = \frac{1}{\tau_1(E)} + \frac{1}{\tau_2(E)} , \tag{1.18}$$

where

$$\tau_1(E) = \sqrt{\frac{m^*}{2}}\ \frac{\ell}{E^{1/2}} , \tag{1.19}$$

$$\tau_2(E) = \frac{2^{3/2}\hbar^2 \Lambda E^{3/2}}{\sqrt{m^*}\ D} \left(\frac{\theta_D}{T}\right) . \tag{1.20}$$

τ_1 and τ_2 are the relaxation times for scattering by impurities and by phonons respectively. For sufficiently high temperatures, $\tau_2^{-1} >> \tau_1^{-1}$ and the electrical and thermal resistance is due almost entirely to the lattice vibrations. At lower temperatures, however, these approximations are no longer valid, a time of relaxation does not exist, and we must find the general solution of the integral equation (1.17).

1.3 The Concept of Formal Relaxation Times

It is now convenient to express (1.17) in a slightly different way. If, following Dingle,[19] we put

$$c(\eta) = -\frac{\hbar}{m^*}\left\{ \left[e\mathcal{E} + T\frac{\partial}{\partial x}\left(\frac{\zeta}{T}\right)\right]\tau(\eta) + \frac{E}{T}\,\frac{\partial T}{\partial x}\,\tau^*(\eta) \right\} , \tag{1.21}$$

then (1.17) splits into two equations:

$$1 = \sqrt{\frac{2}{m^*}}\ \frac{E^{1/2}}{\ell}\,\tau(\eta) + \frac{\sqrt{\frac{1}{2}m^*}}{\hbar^2\Lambda E^{3/2}}\left(\frac{T}{\theta_D}\right)^3 \times$$

$$\int_{-\theta_D/T}^{\theta_D/T} \left\{ E\,\tau(\eta) - \tau(\eta+z)\left[E + \tfrac{1}{2}kTz - D\left(\frac{T}{\theta_D}\right)^2 z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1}\ \frac{z^2\,dz}{|1-e^{-z}|} , \tag{1.22}$$

$$1 = \sqrt{\frac{2}{m^*}}\ \frac{E^{1/2}}{\ell}\,\tau^*(\eta) + \frac{\sqrt{\frac{1}{2}m^*}}{\hbar^2 \Lambda E^{5/2}}\left(\frac{T}{\Theta_D}\right)^3 \times$$

$$\int_{-\Theta_D/T}^{\Theta_D/T} \left\{ E^2 \tau^*(\eta) - \tau^*(\eta+z)\,(E + kTz)\left[E + \tfrac{1}{2}kTz - D\left(\frac{T}{\Theta_D}\right)^2 z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^2\,dz}{|1-e^{-z}|}\,. \tag{1.23}$$

The d.c. electrical conductivity, the thermal conductivity and the thermoelectric effects are given respectively by

$$\sigma = e^2 K_1\,, \qquad K = \frac{K_1 K_3^* - K_2 K_2^*}{K_1\,T}\,, \qquad C = \frac{K_2^* - \zeta K_1}{K_1\,T}\,, \tag{1.24}$$

where

$$K_n = -\frac{16\pi\sqrt{2m^*}}{3h^3}\int E^{n+\frac{1}{2}}\,\tau(\eta)\,\frac{\partial f_0}{\partial \eta}\,d\eta\,, \tag{1.25}$$

$$K_n^* = -\frac{16\pi\sqrt{2m^*}}{3h^3}\int E^{n+\frac{1}{2}}\,\tau^*(\eta)\,\frac{\partial f_0}{\partial \eta}\,d\eta\,. \tag{1.26}$$

Since these expressions are of the same form as those which hold when a time of relaxation exists,[19] τ and τ^* may be regarded as 'formal relaxation times'; at high temperatures each reduces to the relaxation time (1.18), and $\tau^* = \tau$ in any approximation in which terms of order $k\Theta_D/E$ are neglected.

We may also display the above equations in non-dimensional form, similar to that employed by Rhodes.[7] Suppose we make the following definitions:

$$y = \frac{\Theta_D}{T}\,, \tag{1.27}$$

$$\gamma = kT/\varsigma \ , \tag{1.28}$$

$$p = 2^{1/3} \frac{8ma^2}{h^2} \varsigma \left(\frac{\pi}{3}\right)^{2/3} , \tag{1.29}$$

$$\xi = \frac{32}{9\pi} \frac{a}{\ell} \frac{Ma^2 k\Theta_D}{h^2} \frac{\varsigma^2}{c^2} , \tag{1.30}$$

$$\phi(\eta) = \frac{3\pi^2 m^* c^2}{\sqrt{2}\, M k \Theta_D h y p^{3/2}} \tau(\eta) , \tag{1.31}$$

$$\phi^*(\eta) = \frac{3\pi^2 m^* c^2}{\sqrt{2}\, M k \Theta_D h y p^{3/2}} \tau^*(\eta) . \tag{1.32}$$

Then (1.22), (1.23), (1.25) and (1.26) are transformed to

$$\frac{y^4}{2}(1+\gamma\eta)^{3/2} = \xi y^5 (1+\gamma\eta)^2 \phi(\eta)$$
$$+ \int_{-y}^{y} \left\{ p y^2 (1+\gamma\eta)\phi(\eta) - \phi(\eta+z)\left[p y^2 (1+\gamma\eta+\tfrac{1}{2}\gamma z) - z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2 dz}{|1-e^{-z}|} , \tag{1.33}$$

$$\frac{y^4}{2}(1+\gamma\eta)^{5/2} = \xi y^5 (1+\gamma\eta)^3 \phi^*(\eta)$$
$$+ \int_{-y}^{y} \left\{ p y^2 (1+\gamma\eta)^2 \phi^*(\eta) - (1+\gamma\eta+\gamma z)\phi^*(\eta+z)\left[p y^2 (1+\gamma\eta+\tfrac{1}{2}\gamma z) - z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2 dz}{|1-e^{-z}|} , \tag{1.34}$$

$$K_n = -\frac{32 M k \Theta_D P^{3/2} y \, \zeta^{n+\frac{1}{2}}}{9 h^2 \sqrt{m^*} \, c^2 \pi} \int_{-\gamma^{-1}}^{\infty} (1+\gamma\eta)^{n+\frac{1}{2}} \phi(\eta) \frac{\partial f_0}{\partial \eta} d\eta , \quad (1.35)$$

$$K_n^* = -\frac{32 M k \Theta_D P^{3/2} y \, \zeta^{n+\frac{1}{2}}}{9 h^2 \sqrt{m^*} \, c^2 \pi} \int_{-\gamma^{-1}}^{\infty} (1+\gamma\eta)^{n+\frac{1}{2}} \phi^*(\eta) \frac{\partial f_0}{\partial \eta} d\eta . \quad (1.36)$$

To a very good approximation the lower limit of integration in (1.35) and (1.36) may be replaced by $-\infty$.

It may be noted that $P = (\zeta / \zeta_0) \, (2q^2)^{\frac{1}{3}}$ where q is the number of electrons per atom and ζ_0 is the value of ζ at $T = 0$. Except for electrons in a narrow band, $\zeta \simeq \zeta_0$ and P is therefore of order unity.

For a highly degenerate electron gas $\gamma = kT/\zeta$ is small; Rhodes[7] has shown that $k\Theta_D/\zeta$ is approximately 0.003 for a wide range of metals. As is well known, this implies that in calculating the electrical conductivity it is sufficient to retain only the zero-order term in an expansion of $\phi(\eta)$ in rising powers of γ. For the second order effects however - thermal conductivity and thermo-electric effects - it is necessary to retain powers of γ up to γ^2, both in the calculation of $\phi(\eta)$ and $\phi^*(\eta)$ and in the evaluation of integrals (1.35) and (1.36).

Chapter 2

PREVIOUS SOLUTIONS OF THE INTEGRAL EQUATION

A review will now be made of previous attempts to find a solution to the Bloch integral equation. In all instances so far, the solutions which have been derived are to some extent approximate, and most are valid over only part of the possible temperature range. For convenience the various methods will be recast where necessary into a form applicable to the elucidation of the functions ϕ and ϕ^* introduced in the previous chapter, so that the connection between the methods may be most clearly evident. This means that the starting point for the description of each method will be the pair of integral equations (1.33) and (1.34).

2.1. The Bloch High Temperature Approximation

This, the first order approximation to $\phi(\eta)$ and $\phi^*(\eta)$ at high temperatures, was first derived by Bloch.[17] The argument is closely connected with that given in Chapter 1 for the existence of a relaxation time at high temperatures. Since y may be assumed small, we expand all quantities on the R.H.S. of (1.33) and (1.34) in rising powers of z, including the unknown functions $\phi(\eta + z)$ and $\phi^*(\eta + z)$. Retaining only those terms involving the smallest power of z at each stage, (1.33) and (1.34) reduce to the simple algebraic equation

$$\phi^*(\eta) \simeq \phi(\eta) \simeq \frac{(1+\gamma\eta)^{3/2}}{1 + 2\xi y(1+\gamma\eta)^2} . \qquad (2.1)$$

It is now a comparatively trivial matter to evaluate the integrals in (1.35) and (1.36) for a degenerate electron gas, expanding the integrand where necessary in rising powers of the degeneracy parameter γ . The electrical conductivity is found to be proportional to y (i.e. resistivity proportional to T), in agreement with experiment. Because a time of relaxation exists, the Wiedemann - Franz law, relating the thermal and electrical conductivities, is valid.

2.2. The Bloch Interpolation Formula for the Electrical Conductivity

In 1930 Bloch[1] advanced a method for calculating the leading term in the electrical conductivity of a perfectly pure metal at low temperatures which, apparently fortuitously, reproduces approximately the correct form of the high-temperature behaviour as well. It therefore acts as an interpolation formula for the conductivity throughout the entire temperature range.

We first assume that the impurity term ξ and all non-zero powers of γ may be ignored, whereupon (1.33) may be written

$$\rho y^2 \int_{-y}^{y} \left[\phi(\eta)-\phi(\eta+z)\right]\frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^2 dz}{|1-e^{-z}|} = \tfrac{1}{2}y^4 - \int_{-y}^{y}\phi(\eta+z)\,\frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^4\,dz}{|1-e^{-z}|} \, . \qquad (2.2)$$

At low temperatures, we assume that the R.H.S. is small. An approximate solution is then ϕ = const. Putting

$$\phi(\eta) = \alpha + \beta(\eta) + \gamma(\eta) + \cdots \qquad (2.3)$$

where each term is assumed much smaller than the previous one, the method of successive approximations yields:

$$\rho y^2 \int_{-y}^{y} \left[\beta(\eta)-\beta(\eta+z)\right]\frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^2 dz}{|1-e^{-z}|} = \tfrac{1}{2}y^4 - \alpha\int_{-y}^{y}\frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^4 dz}{|1-e^{-z}|} \, ,$$

$$p\, y^2 \int_{-y}^{y} \left[\gamma(\eta) - \gamma(\eta+z)\right] \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|} = -\int_{-y}^{y} \beta(\eta+z) \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^4\,dz}{|1-e^{-z}|}\ , \ \text{etc.} \tag{2.4}$$

For any well - behaved function $F(\eta)$, it is easily shown that

$$\int_{-\infty}^{\infty} \frac{\partial f_0}{\partial \eta}\, d\eta \int_{-y}^{y} \left[F(\eta) - F(\eta+z) \right] \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|} \equiv 0\ . \tag{2.5}$$

It therefore follows from (2.4) that

$$0 = \int_{-\infty}^{\infty} \frac{\partial f_0}{\partial \eta}\, d\eta \left[\tfrac{1}{2} y^4 - \alpha \int_{-y}^{y} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^4\,dz}{|1-e^{-z}|} \right],$$

$$0 = \int_{-\infty}^{\infty} \frac{\partial f_0}{\partial \eta}\, d\eta \int_{-y}^{y} \beta(\eta+z) \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^4\,dz}{|1-e^{-z}|}\ , \quad \text{etc.} \tag{2.6}$$

The first of these determines the leading term α :

$$\begin{aligned}
\tfrac{1}{2} y^4 &= -\alpha \int_{-\infty}^{\infty} \frac{\partial f_0}{\partial \eta}\, d\eta \int_{-y}^{y} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^4\,dz}{|1-e^{-z}|} \\
&= \alpha \int_{-y}^{y} \frac{dz\, z^4}{|1-e^{-z}|} \int_{-\infty}^{\infty} \frac{d\eta}{(e^{\eta+z}+1)(1+e^{-\eta})} \\
&= \alpha \int_{-y}^{y} \frac{dz\ z^5}{|1-e^{-z}|\,(e^{z}-1)}\ .
\end{aligned} \tag{2.7}$$

Hence

$$\alpha = \tfrac{1}{4}\, y^4 / \mathcal{J}_5(y)\ , \tag{2.8}$$

where

$$\mathcal{J}_n(y) = \int_0^y \frac{z^n dz}{(1-e^{-z})(e^z-1)} \quad . \tag{2.9}$$

The second and following equations are subsidiary conditions imposed on the higher order terms $\beta(\eta)$, $\gamma(\eta)$ etc., which are presumed to be solved from eqs.(2.4).

At low temperatures $\mathcal{J}_5(y) \simeq \mathcal{J}_5(\infty) = 124.43$ (see Wilson[18] p.336) so that ϕ ($\simeq \alpha$) is proportional to y^4. With (1.24) and (1.35), this implies that the conductivity σ is proportional to y^5, confirmed by the observed proportionality of the resistivity to T^5. At high temperatures, on the other hand, the leading term in $\mathcal{J}_5(y)$ expanded in rising powers of y is $\frac{1}{4}y^4$ so that $\phi \simeq 1$, in agreement with (2.1). Thus, though conceived as an approximation valid at low temperatures only, (2.8) duplicates the previously derived variation with <u>high</u> temperatures and therefore serves as an interpolation formula yielding correct order-of-magnitude results at all temperatures.

To complete the argument we must justify retrospectively the assumption $\alpha \gg \beta \gg \gamma$ --- . Inspection of (2.4) reveals that at sufficiently low temperatures ($y \to \infty$), $\beta(\eta)$ must be proportional to y^2, compared with the variation of α with y^4. Further, $\gamma(\eta) = O(\beta / y^2)$ etc., so that the series (2.3) is one in descending powers of y^2.

The major weakness of this method is the lack of any obvious way to find the second and higher order terms $\beta(\eta)$, $\gamma(\eta)$ ..., even though the temperature dependence of these functions may be roughly estimated. This is a major limitation, since it means the second-order transport coefficients (thermal conductivity etc.) cannot be investigated.

2.3 Elucidation of the Second Order Terms

The first attempt to find the second order terms in $\phi(\eta)$ at high temperatures was made by Brillouin.[42] Unfortunately the method he evolved is erroneous as well as vastly complicated, but it is instructive to see why.

Brillouin expanded all quantities in the integrand of (1.33) in rising powers of z, and simultaneously all functions of η in rising powers of η . Included in the latter group was

$$\phi(\eta) = \phi(0) + \eta\,\phi'(0) + \tfrac{1}{2}\eta^2\,\phi''(0) + \cdots \qquad (2.10)$$

Equating powers of η on the two sides of the equation, expressions for $\phi(0)$, $\phi'(0)$.... are found, each in the form of a series in rising powers of y . In practice Brillouin evaluated only the terms up to and including $\phi''(0)$, such was the complexity of the mathematics, and with these he calculated the transport coefficients.

The flaw in the argument lies in the expansion of $\phi(\eta)$ in rising powers of η , as Wilson[2] has pointed out. This expansion makes it necessary to apply the well-known asymptotic formula

$$-\int_{-\infty}^{\infty} f(\eta)\,\frac{\partial f_0}{\partial \eta}\,d\eta = f(0) + \frac{\pi^2}{6}f''(0) + \frac{7\pi^4}{360}f''''(0) + \cdots \qquad (2.11)$$

in the evaluation of the integral K_n in (1.35). But the terms on the R.H.S. of (2.11) initially decrease only when successive derivatives $f''(0)$, $f''''(0)$ etc. decrease rapidly, i.e. when $f(\eta)$ is a slowly varying function of η . This requirement is satisfied for the first order approximation to $\phi(\eta)$ expanded in rising powers of y . [From (2.1) this quantity is $(1+\gamma\eta)^{3/2}$.] But the second and higher order coefficients, considered as unexpanded functions of η , do not satisfy the condition, and so the coefficients of y^{2r} ($r \geqslant 1$) in the final expression for K_n become rapidly diverging asymptotic series when recourse is made to the formula (2.11). This is illustrated by Brillouin's result for the electrical conductivity: neglecting terms of order γ^2,

$$\sigma = \sigma_0 \left[1 + y^2 \left(\frac{1}{9} - \frac{\pi^2}{72} \right) + O(y^4) \right] \tag{2.12}$$

where σ_0 isthe first order approximation. In the second-order (y^2) term, $1/9$ is the contribution to the coefficient from $\phi(0)$, $-\pi^2/72$ that from $\phi''(0)$, and so on. The series which begins $(\frac{1}{9} - \pi^2/72 + \ldots)$ is rapidly divergent and Brillouin's termination of this series at the second term is arbitrary and invalid.

Turning now to more legitimate methods, Wilson[2] has shown how to find the second order terms in $\phi(\eta)$ and $\phi^*(\eta)$ for the two cases (a) pure metals at high temperatures, and (b) impure metals at low temperatures.

The procedure appropriate at high temperatures starts from the observation that, according to (2.1), the first approximation to $\phi(\eta)$ when $\xi = 0$ is

$$\phi_1(\eta) = (1 + \gamma\eta)^{3/2}. \tag{2.13}$$

We now put

$$\phi(\eta) = \phi_1(\eta) + \phi_2(\eta) + \cdots + \phi_n(\eta) + \cdots \tag{2.14}$$

where ϕ_n is obtained by substituting the first n terms of the series for $\phi(\eta)$ in (1.33), making the previously described approximations for the term involving ϕ_n but no approximation for the preceding terms. This gives

$$\phi_n(\eta) = \phi_{n-1}(\eta) - \frac{2}{y^4} \int_{-y}^{y} \left\{ \rho y^2 (1+\gamma\eta)\phi_{n-1}(\eta) - \phi_{n-1}(\eta+z)\left[\rho y^2(1+\gamma\eta+\tfrac{1}{2}\gamma z) - z^2\right] \right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|}. \tag{2.15}$$

By a similar argument, the higher order approximations $\phi_2^*(\eta)$, $\phi_3^*(\eta)$..... may be found for the function $\phi^*(\eta)$.

Since $\phi_1(\eta)$ is of extremely simple form, $\phi_2(\eta)$ is reasonably straightforward to evaluate and can, if desired, be expanded in rising powers of y. The higher order terms ϕ_3, ϕ_4,... are, in principle, calculable from (2.15), but the labour required increases rapidly and Wilson contented himself with the evaluation of ϕ_2. This is quite sufficient, so long as only the second order terms in the transport coefficients are required, but termination of the process at this early stage rules out any possibility of investigating the convergence of the series (2.14) or of the resulting series for ϕ in rising powers of y.

As Wilson pointed out in his paper, it is more straightforward, oddly enough, to calculate the contribution to the integrals K_n and K_n^* in (1.35) and (1.36) from the higher order terms ϕ_n and ϕ_n^* ($n \geq 2$) than it is to calculate the ϕ's themselves, if the main interest lies in the transport coefficients. This is because, in the resulting double integrals over η and z, the integration over η can be transformed by the identity

$$\int_{-\infty}^{\infty} \frac{F(\eta)\, d\eta}{(e^{-\eta}+1)(e^{\eta+z}+1)} \equiv - \frac{1}{e^{z}-1} \int_{-\infty}^{\infty} \left[G(\eta) - G(\eta - z) \right] \frac{\partial f_0}{\partial \eta}\, d\eta , \quad (2.16)$$

where

$$G(\eta) = \int^{\eta} F(\eta')\, d\eta' . \quad (2.17)$$

Application of this, followed by the expansion where necessary of functions of γ in rising powers of γ, enables the integration over η to be carried out resulting in expressions for K_n and K_n^* in terms of the family of integrals $\mathcal{J}_n(y)$ of (2.9). It is then straightforward to calculate the transport coefficients up to the second order terms - those of order γ^2 and y^2.

For an impure metal ($\xi \neq 0$) at low temperatures, the dominant term on the R.H.S. of (1.33) and (1.34) is the one involving ξ . Physically this means that, in this range of temperature, scattering by impurities predominates over scattering by phonons. The first approximation to ϕ under these circumstances is therefore

$$\phi_1(\eta) = \left[2y\xi\sqrt{1+\gamma\eta} \right]^{-1} . \tag{2.18}$$

Once again an expansion of $\phi(\eta)$ is made of the same form as (2.14), where ϕ_n is now determined by

$$0 = \xi y^5 (1+\gamma\eta)^2 \phi_n(\eta)$$
$$+ \int_{-y}^{y} \left\{ \rho y^2 (1+\gamma\eta)\phi_{n-1}(\eta) - \phi_{n-1}(\eta+z)\left[\rho y^2(1+\gamma\eta+\tfrac{1}{2}\gamma z) - z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \; \frac{z^2\,dz}{|1-e^{-z}|} . \tag{2.19}$$

The expansion for $\phi(\eta)$ is therefore in descending powers of the impurity parameter ξ . As before, it is not too difficult to calculate $\phi_2(\eta)$ (and correspondingly $\phi_2^*(\eta)$) and hence, by a similar process to the one described above, find the second order terms for the transport coefficients. The process has been taken one stage further by Dube[41] who calculated $\phi_3(\eta)$ in order to test the validity of Matthiessen's rule, but the labour involved in further continuation would obviously be out of proportion to the results achieved. There is therefore the same difficulty as before, namely that the convergence of the series for ϕ cannot be investigated; in addition, the method cannot be applied at all to the case of a pure metal.

2.4. The Numerical Method of Rhodes

In 1950 Rhodes[7] pointed out that a much better high-temperature approximation than the one obtained by Bloch[17] could be found by taking $\phi(\eta + z) \simeq \phi(\eta)$ in (1.33), ignoring the small term $\frac{1}{2}\gamma z$ but keeping the rest of the integrand unaltered. Putting $\xi = 0$, the first approximation to $\phi(\eta)$ for a pure metal is then

$$\phi_1(\eta) = \frac{\frac{1}{2}y^4(1+\gamma\eta)^{3/2}}{\int_{-y}^{y}\frac{e^{\eta}+1}{e^{\eta+z}+1}\frac{z^4\,dz}{|1-e^{-z}|}} . \tag{2.20}$$

Expanding the integrand in the denominator in rising powers of z, integration of the leading term only yields directly the first approximation to ϕ found by Bloch. Significantly, however, (2.20) also exhibits the same variation with y (viz. $\sim y^4$) as the Bloch low temperature solution (2.8), and might therefore be expected to be valid over a much greater range of temperature than (2.1).

Rhodes devised the following method of successive approximations for the calculation of the (almost) exact function $\phi(\eta)$, starting from ϕ_1. The integral equation (1.33) is first rewritten in the form

$$\rho y^2(1+\gamma\eta)\phi_{\nu+1}(\eta)\int_{-y}^{y}\frac{e^{\eta}+1}{e^{\eta+z}+1}\frac{z^2\,dz}{|1-e^{-z}|} = \frac{1}{2}y^4(1+\gamma\eta)^{3/2}$$

$$+\int_{-y}^{y}\phi_\nu(\eta+z)\left[\rho y^2\left(1+\gamma\eta+\tfrac{1}{2}\gamma z\right)-z^2\right]\frac{e^{\eta}+1}{e^{\eta+z}+1}\frac{z^2\,dz}{|1-e^{-z}|} , \tag{2.21}$$

where the subscripts ν and $\nu + 1$ identify the particular approximation to $\phi(\eta)$ under consideration. Starting with $\nu = 1$, the procedure is to insert $\phi_\nu(\eta)$ into the R.H.S. of (2.21) and, for fixed values of γ and ρ and for a limited number of values of y, calculate numerically the next approximation $\phi_{\nu+1}(\eta)$. This process is repeated until $\phi_{\nu+1}$ agrees with ϕ_ν to within 1% for all values of η up to $\eta \doteq 5$.

Rhodes found that in practice $\phi_1(\eta)$ was a sufficiently good approximation for $y \lesssim 1$, confirming the original expectation that ϕ_1 would be valid over a wide range of values of y. For $y > 1$, higher approximations are required, the number of such approximations increasing approximately linearly with y up to $y = 5$. Having elucidated the numerical form of $\phi(\eta)$, Rhodes was able to integrate numerically the K_1 integral of (1.35) to find the electrical conductivity, whose temperature dependence could then be compared with experiment over almost the whole temperature range.

In principle this method may be extended to the calculation of $\phi^*(\eta)$ and consequent evaluation of the second order transport coefficients. Compared with the previously outlined techniques, it has the considerable merit of exhibiting explicitly the numerical variation of ϕ (and ϕ^*) with η, as an intermediate step in the determination of the electrical conductivity etc. On the other hand this is not as satisfactory as would be analytic knowledge of the functions concerned, and the numerical variation of ϕ with temperature (except in the region $y < 1$) can in any case be obtained only after considerable labour.

2.5. Application of a Variational Principle

Starting once again from (1.33), we define a linear operator L by

$$L(\phi) \equiv \xi y^5 (1+\gamma\eta)^2 \phi(\eta)$$
$$+ \int_{-y}^{y} \left\{ \rho y^2 (1+\gamma\eta)\,\phi(\eta) - \phi(\eta+z)\left[\rho y^2\left(1+\gamma\eta+\tfrac{1}{2}\gamma z\right) - z^2\right]\right\} \frac{e^{\eta}+1}{e^{\eta+z}+1}\,\frac{z^2\,dz}{|1-e^{-z}|}\,, \tag{2.22}$$

whereupon (1.33) reduces to

$$L(\phi) = \tfrac{1}{2} y^4 (1+\gamma\eta)^{3/2}. \tag{2.23}$$

Kohler[5,6] has shown that the solution $\phi(\eta)$ is such that the integral

$$\int_{-\infty}^{\infty} \phi(\eta)\, L(\phi)\, \frac{\partial f_0}{\partial \eta}\, d\eta \tag{2.24}$$

is a maximum, subject to the subsidiary condition

$$\int_{-\infty}^{\infty} \phi(\eta)\, L(\phi)\, \frac{\partial f_0}{\partial \eta}\, d\eta = \tfrac{1}{2} y^4 \int_{-\infty}^{\infty} \phi(\eta)(1+\gamma\eta)^{3/2} \frac{\partial f_0}{\partial \eta}\, d\eta . \tag{2.25}$$

Similar relations hold for $\phi^*(\eta)$, a slightly different operator L^* being defined in the obvious way from the R.H.S. of (1.34).

Armed with this information, it is now possible to assume a trial form for the unknown functions $\phi(\eta)$ and $\phi^*(\eta)$ and to apply the variational principle above to determine the coefficients. Kohler[5,6] and, later, Sondheimer[3] have each assumed a power series expansion

$$\phi(\eta) = \sum_{\mu=0}^{\infty} \phi_\mu \eta^\mu , \tag{2.26}$$

whereupon application of the variational principle leads to

$$\sum_{\nu=0}^{\infty} d_{\mu\nu}\, \phi_\nu = \alpha_\mu \tag{2.27}$$

where

$$d_{\mu\nu} = \int_{-\infty}^{\infty} \eta^\mu L(\eta^\nu) \frac{\partial f_0}{\partial \eta}\, d\eta , \tag{2.28}$$

$$\alpha_\mu = \tfrac{1}{2} y^4 \int_{-\infty}^{\infty} (1+\gamma\eta)^{3/2} \eta^\mu \frac{\partial f_0}{\partial \eta}\, d\eta . \tag{2.29}$$

(Eq. (2.27) had earlier been derived by Kroll[43] but without proper theoretical justification).

The solution of (2.27) for the coefficients ϕ_p clearly involves a quotient of infinite determinants whose elements are the $\alpha_{p\nu}$ and α_p defined above. These quantities may be evaluated for a degenerate electron gas (for which asymptotic expansions in rising powers of γ are permissible) although the final expression for $\alpha_{p\nu}$ is rather complicated.

After the evaluation of the integrals (1.35) and (1.36) by the usual methods, it is an exercise in the manipulation of infinite determinants to derive final expressions for the transport coefficients of interest. Kohler evaluated explicitly only the terms of lower order, and the first full development of the method was carried through by Sondheimer, whose work has been regarded for the last two decades as providing the most satisfactory general solution of the Bloch integral equation so far obtained.

Nevertheless, a substantial measure of unease persists regarding the validity of the method. Since there is no initial guarantee that the exact solution $\phi(\eta)$ can be expanded as a power series in η, it is possible that the variational method is picking out only the best-fit solution, selected from that class of functions which can legitimately be expressed in this form. Again, it is unsatisfactory that no discussion can be given of the convergence of the power series in question, or of the convergence of the infinite determinants. Breaking off the determinants at a finite number of rows and columns (inevitable sooner or later if a numerical result is finally to be obtained) is equivalent to the termination of the power series as a polynomial, and no estimate can be given of the error involved in ignoring the remainder. Hence, although the transport coefficients derived are in generally good agreement with experimental values, there could still be a substantial difference between the real functions $\phi(\eta)$ and $\phi^*(\eta)$ and the approximations to these functions which are derived and employed in the way described here.

Doubts about the validity of the variational method are reinforced by the strong evidence for its partial failure when applied to the problem of polar semiconductors. Here the integral equation reduces to a difference equation, due to the phonons of the optical mode having but a single frequency. The difference equation has been solved by Howarth and Sondheimer[4] using essentially the same variational argument as for metals. For the degenerate case, their results for the electrical conductivity and thermoelectric power disagree up to 15% with the numerical calculations of Delves[44] over a selected range of temperature. At low temperatures they are also in marked disagreement with the corresponding expressions calculated by Durney[45] by an iterative method.

Chapter 3

FORMAL EXPANSION OF THE SOLUTION AS A DOUBLE SERIES

3.1. Further Simplification of the Integral Equation

The ensuing analysis is simplified by the smallness of γ - typically, of order 10^{-3}. To evaluate physical quantities of interest, it is necessary only to retain terms up to second order in the expansion of $\phi(\eta)$ and $\phi^*(\eta)$ in rising powers of γ. Indeed if only the electrical conductivity is required, an excellent approximation is obtained by taking the degeneracy limit $\gamma \to 0$, in which case both (1.33) and (1.34) reduce to the same equation

$$\frac{1}{2} y^4 = \xi y^5 \phi(\eta) + \int_{-y}^{y} \left\{ \rho y^2 \phi(\eta) - \phi(\eta+z)\left[\rho y^2 - z^2\right] \right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|} . \tag{3.1}$$

The solution of this equation is an even function of η. This may be proved by returning to (1.33), expanding $(1 + \gamma\eta)^{3/2}$ by the binomial theorem in rising powers of $\gamma\eta$, expressing $\phi(\eta)$ as the sum of an even and an odd function of η, and equating the even and odd functions on the two sides of the equation. The equation derived from the equality of the odd functions reduces in the limit $\gamma = 0$ to a homogeneous integral equation for the odd function ϕ_{odd}, whose only acceptable solution is $\phi_{odd}(\eta) = 0$. This agrees with the numerical calculation by Rhodes[7] who found that for a small but non-zero value of γ the function $\phi(\eta)$ is <u>very nearly</u> even; and likewise with the results of Sondheimer's analysis[3], in which $\gamma = 0$

nullifies the coefficients of odd powers of η in the trial expansion of $\phi(\eta)$.

For the time being we shall assume $\xi = 0$, i.e. no impurity scattering. The equation to be solved then takes the elemental form

$$\frac{1}{2}y^4 = \int_{-y}^{y} \left\{ \rho y^2 \phi(\eta) - \phi(\eta+z)\left[\rho y^2 - z^2\right] \right\} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^2\,dz}{|1-e^{-z}|} . \qquad (3.2)$$

Attention will now be directed towards finding a solution of this equation, hopefully valid at both high and low temperatures. Consideration will later be given to the applicability of similar methods to the more general equations (3.1), (1.33) and (1.34).

3.2. Double Series Expansion for ϕ Suggested by the Method of Successive Approximations

We recall that the first order approximation to $\phi(\eta)$ adopted by Rhodes[7] was obtained by taking $\phi(\eta+z) \simeq \phi(\eta)$ in (3.2) and leaving the rest of the integrand unaltered. This approximation ϕ_1 is therefore

$$\phi_1(\eta) = \frac{1}{2}y^4 \left[\int_{-y}^{y} \frac{e^{\eta}+1}{e^{\eta+z}+1} \frac{z^4\,dz}{|1-e^{-z}|} \right]^{-1} . \qquad (3.3)$$

The expression on the R.H.S. may be converted to an infinite series in rising even powers of y by expanding the integrand in rising powers of z, carrying out the integration and then inverting the resulting series. The result is

$$\phi_1(\eta) = 1 + y^2\left[-\frac{1}{18} + \frac{2}{3}(1+e^{\eta})^{-1} - \frac{2}{3}(1+e^{\eta})^{-2}\right]$$
$$+ y^4\left[\frac{49}{12960} + \frac{1}{108}(1+e^{\eta})^{-1} - \frac{7}{108}(1+e^{\eta})^{-2} + \frac{1}{9}(1+e^{\eta})^{-3} - \frac{1}{18}(1+e^{\eta})^{-4}\right] + O(y^6) \qquad (3.4)$$

Corrections to this first approximation may be made by solving (3.2) by the method of successive approximations. When added to (3.4), their effect is to change the numerical values of the coefficients of the various powers of $(1+e^{\eta})^{-1}$ which appear, but not the <u>form</u> of the expression. We may assume therefore that the exact function $\phi(\eta)$ may be expanded as a series in rising powers of y^2, the coefficients being polynomials of successively higher degree in the variable $(1+e^{\eta})^{-1}$.

At this juncture it is obviously preferable to make an explicit change of variable from η to

$$x = (1+e^{\eta})^{-1} \tag{3.5}$$

which ranges between 1 and 0 as η runs from $-\infty$ to ∞. As a consequence, we must write

$$\phi(\eta) = \psi(x) \tag{3.6}$$

and our assumption is that ψ can be expanded in the form

$$\psi(x) = \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{2r} a_s^r x^s \tag{3.7}$$

where the a_s^r are pure numbers. We assume nothing about the convergence or otherwise of this series; this issue will be investigated in due course. It is worth noting that in the limit $y = 0$ the integral K_n given by (1.35) now looks like

$$K_n = \frac{32 M k \Theta_0 P^{3/2} y \, \zeta^{n+\frac{1}{2}}}{9 h^2 \sqrt{m^*} \, C^2 \pi} \int_0^1 \psi(x)\, dx \quad ; \tag{3.8}$$

in the same limit, K_n^* is identical to this.

3.3. Recurrence Relation for the Coefficients a_s^r

A recurrence relation which generates the numbers a_s^r may be found as follows. First, we transform (3.2) by the substitution (3.5) to

$$\frac{1}{2} y^4 = \int_{-y}^{y} \frac{dz\ z^2}{[x + e^{z}(1-x)]\,|1-e^{-z}|} \left\{ p y^2 \psi(x) - (p y^2 - z^2)\, \psi\left[\frac{x}{x + e^{z}(1-x)}\right] \right\}. \tag{3.9}$$

Expanding $\psi(x)$ in accordance with (3.7),

$$\frac{1}{2} y^4 = \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{2r} a_s^r x^s \int_{-y}^{y} \frac{dz\ z^2}{|z|} \left(\frac{-z}{e^{-z}-1}\right) \left\{ \frac{p y^2}{x + e^{z}(1-x)} - \frac{p y^2 - z^2}{[x + e^{z}(1-x)]^{s+1}} \right\}. \tag{3.10}$$

Now

$$\frac{-z}{e^{-z} - 1} = \sum_{p=0}^{\infty} \frac{B_p (-z)^p}{p!} \tag{3.11}$$

where B_p is the p th Bernoulli number, while expansion of the other factors is facilitated by the general formula due to Schlömilch[39] (see also Jordan[39]) for the expansion of any function of e^z in rising powers of z :

$$u(e^z) = \sum_{m=0}^{\infty} \frac{z^m}{m!} \sum_{\nu=0}^{m} C_m^{\nu} \left(\frac{d^{\nu} u}{d y^{\nu}}\right)_{y=1} \tag{3.12}$$

where C_m^{ν} is a Stirling number of the second kind, and $y = e^z$. Hence

$$[x + e^{z}(1-x)]^{-n} = \sum_{m=0}^{\infty} \frac{z^m}{m!} \sum_{\nu=0}^{m} C_m^{\nu} (-1)^{\nu} \frac{(n+\nu-1)!}{(n-1)!} (1-x)^{\nu} . \tag{3.13}$$

The present theory calls for the product of (3.11) and (3.13) with n taking the values 1 and $s + 1$ in turn. The general product is

$$\left(\frac{-z}{e^{-z}-1}\right)[x+e^{z}(1-x)]^{-n} = \sum_{\ell=0}^{\infty} \frac{z^\ell}{\ell!}(-1)^\ell \sum_{m=0}^{\ell} \binom{\ell}{m}(-1)^m B_{\ell-m} \sum_{\upsilon=0}^{m} C_m^\upsilon (-1)^\upsilon \frac{(n+\upsilon-1)!}{(n-1)!}(1-x)^\upsilon$$

$$= \sum_{\ell=0}^{\infty} \frac{z^\ell}{\ell!}(-1)^\ell \sum_{\upsilon=0}^{\ell}(-1)^\upsilon \frac{(n+\upsilon-1)!}{(n-1)!}(1-x)^\upsilon \sum_{m=\upsilon}^{\ell} \binom{\ell}{m}(-1)^m B_{\ell-m}\, C_m^\upsilon \;, \tag{3.14}$$

$\binom{\ell}{m}$ being the binomial coefficient $\ell!/[m!(\ell-m)!]$. Now

$$\sum_{m=\upsilon}^{\ell} \binom{\ell}{m}(-1)^m B_{\ell-m}\, C_m^\upsilon = (-1)^\ell \frac{\ell}{\upsilon} C_\ell^\upsilon \;, \quad \upsilon \neq 0 \,. \tag{3.15}$$

This result does not appear to be generally known, and a proof of it is given in Appendix 1. When $\upsilon = 0$ the summation is trivial since, by convention,

$$\begin{aligned} C_m^0 &= 1 \;, \; m = 0 \,, \\ &= 0 \;, \; m \geq 1 \,. \end{aligned} \tag{3.16}$$

Hence, provided we interpret $(\ell/\upsilon)\, C_\ell^\upsilon$ to mean $(-1)^\ell B_\ell$ when $\upsilon = 0$,

$$\left(\frac{-z}{e^{-z}-1}\right)[x+e^{z}(1-x)]^{-n} = \sum_{\ell=0}^{\infty} \frac{z^\ell}{\ell!} \sum_{\upsilon=0}^{\ell} (-1)^\upsilon \frac{(n+\upsilon-1)!}{(n-1)!} \frac{\ell}{\upsilon} C_\ell^\upsilon (1-x)^\upsilon \,. \tag{3.17}$$

With this result we may return now to (3.10) which on substitution becomes

$$\frac{1}{2}\, y^4 = \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{2r} a_s^r x^s \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \sum_{\upsilon=0}^{\ell} (-1)^\upsilon \frac{\ell}{\upsilon} C_\ell^\upsilon (1-x)^\upsilon \int_{-y}^{y} \frac{dz\, z^{\ell+2}}{|z|} \left\{ \rho y^2 \upsilon! - (\rho y^2 - z^2)\frac{(\upsilon+s)!}{s!} \right\}$$

$$= 2\sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{2r} a_s^r x^s \sum_{\ell=0,2,4\ldots}^{\infty} \frac{y^{\ell+4}}{\ell!} \sum_{\upsilon=0}^{\ell} (-1)^\upsilon \upsilon! \frac{\ell}{\upsilon} C_\ell^\upsilon (1-x)^\upsilon \left\{ \frac{\rho}{\ell+2} - \binom{\upsilon+s}{\upsilon}\left(\frac{\rho}{\ell+2} - \frac{1}{\ell+4}\right)\right\}$$

$$= \tfrac{1}{2}y^4 \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{2r} a_s^r x^s \sum_{t=0}^{\infty} \frac{y^{2t}}{(2t)!} \sum_{\nu=0}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} (1-x)^\nu \left\{ \frac{4p}{2t+2} - \binom{\nu+s}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\right\}$$

$$= \tfrac{1}{2}y^4 \sum_{n=0}^{\infty} y^{2n} \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{s=0}^{2n-2t} a_s^{n-t} x^s \sum_{\nu=0}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} (1-x)^\nu \left\{ \frac{4p}{2t+2} - \binom{\nu+s}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\right\}.$$

(3.18)

Hence, equating coefficients of powers of y,

$$a_0^0 = 1 \tag{3.19}$$

and, for n=1,2,3,.....,

$$0 = \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{s=0}^{2n-2t} a_s^{n-t} x^s \sum_{\nu=0}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} \sum_{r=0}^{\nu} \binom{\nu}{r} (-x)^r \left\{ \frac{4p}{2t+2} - \binom{\nu+s}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\right\}$$

$$= \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{s=0}^{2n-2t} a_s^{n-t} x^s \sum_{r=0}^{2t} (-x)^r \sum_{\nu=r}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} \binom{\nu}{r} \left\{ \frac{4p}{2t+2} - \binom{\nu+s}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\right\}$$

$$= \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{\ell=0}^{2n} x^\ell \sum_{r=0,\,\ell-2n+2t}^{2t,\,\ell} (-1)^r a_{\ell-r}^{n-t} \sum_{\nu=r}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} \binom{\nu}{r} \left\{ \frac{4p}{2t+2} - \binom{\nu+\ell-r}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\right\},$$

(3.20)

where $\sum\limits_{r=a,b}^{c,d}$ means that r runs from the greater of a and b to the lesser of c and d. For ℓ =0,1,2,..2n, the coefficient of x^ℓ must be zero, from which follows

$$a_\ell^n = \sum_{t=1}^{n} \frac{1}{(2t)!} \sum_{r=0,\,\ell-2n+2t}^{2t,\,\ell} (-1)^r a_{\ell-r}^{n-t} \sum_{\nu=r}^{2t} (-1)^\nu \nu! \, \frac{2t}{\nu} C_{2t}^{\nu} \binom{\nu}{r} \left\{ \binom{\nu+\ell-r}{\nu}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right) - \frac{4p}{2t+2}\right\}.$$

(3.21)

The R.H.S. of this equation may be simplified through the equality

$$\sum_{\nu=r}^{2t} (-1)^{\nu} \nu! \, \frac{2t}{\nu} \, C_{2t}^{\nu} \binom{\nu+s}{r+s} = \sum_{\nu=r}^{s+r,\,2t} \nu! \, \frac{2t}{\nu} \, C_{2t}^{\nu} \binom{s}{\nu-r} \tag{3.22}$$

derived in Appendix 1. The recurrence relation (3.21) then reduces to

$$a_{\ell}^{n} = \sum_{t=1}^{n} \sum_{r=0,\,\ell-2n+2t}^{2t,\,\ell} (-1)^{r} a_{\ell-r}^{n-t} \left\{ \left(\frac{4p}{2t+2} - \frac{4}{2t+4} \right) \binom{\ell}{r} \sum_{\nu=r}^{2t,\,\ell} \frac{\nu!}{(2t)!} \, \frac{2t}{\nu} \, C_{2t}^{\nu} \binom{\ell-r}{\nu-r} - \frac{4p}{2t+2} \, \frac{r!}{(2t)!} \, \frac{2t}{r} \, C_{2t}^{r} \right\} \tag{3.23}$$

It does not appear possible to express the remaining ν -summation in any more concise form (see Appendix 1) and (3.23) is therefore the simplest generator of the general coefficient a_{ℓ}^{n} starting from $a_{0}^{0} = 1$.

Chapter 4

APPROXIMATE SOLUTIONS FOR THE COEFFICIENTS a_0^n AND a_{2n}^n

The recurrence relation (3.23) for a_ℓ^n looks considerably simpler at the two ends of the range for ℓ , viz. $\ell = 0$ and $\ell = 2n$. It is then possible to establish approximate solutions for the two coefficients in question.

4.1 Approximate Solution for a_0^n

Putting $\ell = 0$ in (3.23), the recurrence relation reduces to

$$a_0^n = -\sum_{t=1}^{n} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} a_0^{n-t}, \tag{4.1}$$

i.e.

$$0 = \sum_{t=0}^{n} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} a_0^{n-t}. \tag{4.2}$$

Since this equation is true for all $n \geqslant 1$,

$$0 = \sum_{n=1}^{\infty} x^n \sum_{t=0}^{n} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} a_0^{n-t}, \tag{4.3}$$

where x is any variable. Adding 1 to both sides,

$$\begin{aligned} 1 &= \sum_{n=0}^{\infty} x^n \sum_{t=0}^{n} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} a_0^{n-t} \\ &= \sum_{t=0}^{\infty} \sum_{s=0}^{\infty} x^{t+s} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} a_0^{s} \quad . \end{aligned} \tag{4.4}$$

The summations over s and t may now be separated, yielding

$$\sum_{s=0}^{\infty} a_0^s \, x^s = 1 / S(x) \tag{4.5}$$

where

$$S(x) = \sum_{t=0}^{\infty} x^t \frac{B_{2t}}{(2t)!} \frac{4}{2t+4}$$

$$= 1 + \frac{x}{18} - \frac{x^2}{1440} + \frac{x^3}{75600} - \frac{x^4}{3628800} + \cdots . \tag{4.6}$$

It is not possible to express the function $S(x)$ in closed form, although it is easily shown that it may be represented by the integral

$$S(x) = \frac{64}{x^2} \int_0^{\frac{1}{2}x^{1/2}} z^4 \coth z \, dz . \tag{4.7}$$

It follows from the Darboux theorem[31] that the late terms in the expansion of $1 / S(x)$ in rising powers of x are determined by the position of the singularity of this function which is nearest the origin. This means that, when s is large, a_0^s is determined by the zero of $S(x)$ lying nearest the origin. From the definition (4.6), it is evident that this zero is located along the negative real axis, and its value can be found with reasonable precision by truncating the series and finding the smallest zero of the resulting polynomial. Retaining all terms up to x^{15}, it is easily shown that the zero in question is at $x = -14.391169$ (correct to the last figure quoted), dS/dx at that point being 0.08911099. Hence in the neighbourhood of this zero,

$$S(x) \simeq 0.08911099 \, (x + 14.391169). \tag{4.8}$$

Expanding the reciprocal of this expression in rising powers of x, we see from (4.5) that, for large s,

$$a_0^s \simeq \frac{0.7797810}{(-14.391169)^s} \quad . \tag{4.9}$$

It should be pointed out that (4.5) could have been derived much more directly by putting $x = 0$ in (3.9). This leads to

$$\psi(0) = \tfrac{1}{2} y^4 \left[\int_{-y}^{y} \frac{dz \; z^4}{|e^z - 1|} \right]^{-1}, \tag{4.10}$$

so that, expanding the integrand on the R.H.S. and carrying out the integration,

$$\sum_{r=0}^{\infty} y^{2r} a_0^r = \left[\sum_{t=0}^{\infty} y^{2t} \frac{B_{2t}}{(2t)!} \frac{4}{2t+4} \right]^{-1} . \tag{4.11}$$

However it is still worthwhile to demonstrate for this simple case the technique of deriving (4.5) from (4.1), for almost the same method must be selected for the much more difficult task of finding the approximate form of the coefficient a_{2n}^n.

4.2. Approximate Solution for a_{2n}^n

Putting $\ell = 2n$ in (3.23), the recurrence relation reduces to

$$b(n) = \sum_{t=1}^{n} b(n-t) \left[\left(\frac{4\rho}{2t+2} - \frac{4}{2t+4} \right) \binom{2n}{2t} - \frac{4\rho}{2t+2} \right] \tag{4.12}$$

where $b(n) = a_{2n}^n$. It may be observed that, for large n, the first term in the square bracket is generally dominant because of the $\binom{2n}{2t}$ factor; for this reason the two terms will be manipulated in slightly different ways.

Since (4.12) is true for all $n \geqslant 1$,

$$\sum_{n=1}^{\infty} \frac{f(n)\,x^n}{(2n)!} = \sum_{n=1}^{\infty} \frac{x^n}{(2n)!} \sum_{t=1}^{n} f(n-t)\left[\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\binom{2n}{2t} - \frac{4p}{2t+2}\right],$$

$$(4.13)$$

where x is any variable. Adding 1 to both sides,

$$\sum_{n=0}^{\infty} \frac{f(n)\,x^n}{(2n)!} = 1 + \sum_{n=1}^{\infty} \frac{x^n}{(2n)!} \sum_{t=1}^{n} f(n-t)\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)\binom{2n}{2t} - 4p \sum_{n=1}^{\infty} \frac{x^n}{(2n)!} \sum_{t=1}^{n} \frac{f(n-t)}{2t+2}$$

$$= 1 + \sum_{t=1}^{\infty} \sum_{s=0}^{\infty} \frac{x^{t+s} f(s)}{(2s)!\,(2t)!}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right) - 4p \sum_{n=1}^{\infty} \frac{x^n}{(2n)!} \sum_{t=1}^{n} \frac{f(n-t)}{2t+2}.$$

$$(4.14)$$

Separating the s and t summations in the second term on the R.H.S. and replacing the dummy suffix s by n,

$$\sum_{n=0}^{\infty} \frac{f(n)\,x^n}{(2n)!} = \frac{1 - 4p \sum_{n=1}^{\infty} \frac{x^n}{(2n)!} \sum_{t=1}^{n} \frac{f(n-t)}{2t+2}}{1 - \sum_{t=1}^{\infty} \frac{x^t}{(2t)!}\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right)}.$$

$$(4.15)$$

We denote by $S_p(x)$ the function defined by the denominator of (4.15). Once again it follows from the Darboux theorem[31] that the late terms in the expansion of the R.H.S. of (4.15) in rising powers of x are determined by the position of the singularity which is nearest the origin, i.e. by the smallest zero of the function $S_p(x)$. On this occasion it is possible to find a closed expression for our function, since the two summations involved are both essentially of the type

$$\sum_{t=0}^{\infty} \frac{z^{2t}}{(2t)!\,(2t+r)} = z^{-r} \int_0^z \cosh z \; z^{r-1}\, dz,$$

$$(4.16)$$

which is easily integrated by parts. Thus

$$S_p(x) = 2p + \frac{4}{z^4}\left[(1-p)z^3 \sinh z - (3-p)z^2 \cosh z + 6z \sinh z - 6\cosh z + 6 - pz^2\right] \tag{4.17}$$

where $z^2 = x$. It is now a straightforward procedure to determine the smallest zero of $S_p(x)$ to any desired accuracy for a specified value of p.

The value of the parameter p is determined mainly by the number of free electrons per atom and is never very different from unity. (see § 1.3). For monovalent metals, p is approximately 1.25 and this value has been assigned to p (for the time being) whenever necessary.

From the definition of $S_p(x)$ it is obvious that the zero of $S_{1.25}(x)$ lying nearest the origin is located along the positive real axis. It is easily shown that its value is x_0=2.97710300694449.... and that $dS_{1.25}/dx$ at that point is -0.383123945939860. In the neighbourhood of this zero, it follows that

$$S_{1.25}(x) = 0.383123945939860\,(x_0 - x) \tag{4.18}$$

Hence, when n is large,

$$\frac{f(n)}{(2n)!} \simeq \frac{A}{1.14059945148999\; x_0^n} \tag{4.19}$$

where

$$A = 1 - 5\sum_{n=1}^{\infty} \frac{x_0^n}{(2n)!} \sum_{t=1}^{n} \frac{f(n-t)}{2t+2}, \tag{4.20}$$

assuming that this sum converges.

For reasonably small values of n, say up to n = 6, the summation contributions in (4.20) may be calculated by hand, inserting the exact values of $f(n)$ found from (4.12) with p = 1.25.

Although the latter * increase rapidly with n [in accordance with our prediction (4.19)] , the contributions to the sum in (4.20) decrease fairly rapidly, from 0.3721 for n = 1 to -0.0035 for n=6. For larger values of n, it is good enough to include only the t=1 contribution in the t-summation, and approximate $f(n-1)$ through (4.19). The equation which determines A is therefore

$$A \simeq 1 - 5\sum_{n=1}^{6} \frac{x_0^n}{(2n)!}\sum_{t=1}^{n}\frac{f(n-t)}{2t+2} - \frac{5}{4}\,\frac{x_0\,A}{1.1405994514 8999}\sum_{n=7}^{\infty}\frac{1}{2n(2n-1)}, \tag{4.21}$$

the summation over n in the final term having the value 0.0399365023492673. Solving for A, we find A= -0.60126, which yields -0.52715 for the value of the multiplying constant in (4.19). Due to the approximations made during the calculation, this value agrees with the exact one only to the first two decimal places, as will be demonstrated in the next chapter.

It is convenient at this point to evaluate the second order term in a_{2n}^n which will be required for the analysis of Chapter 8. Substituting

$$a_{2n}^n \propto \frac{(2n)!}{x^n}\left[1 + \frac{c}{2n} + \frac{d}{2n(2n-1)} + \cdots\right] \tag{4.22}$$

in (4.12), extending the t-summation to t=∞ and multiplying throughout by $x^n/(2n)!$,

$$1 + \frac{c}{2n} + \frac{d}{2n(2n-1)} + \cdots = \sum_{t=1}^{\infty}\frac{x^t}{(2t)!}\left(\frac{4P}{2t+2} - \frac{4}{2t+4}\right)\left[1 + \frac{c}{2n-2t} + \frac{d}{(2n-2t)(2n-2t-1)} + \cdots\right]$$
$$- \frac{Px}{2n(2n-1)}\left[1 + \frac{c}{2n-2} + \cdots\right] + O\left(\frac{1}{n^4}\right). \tag{4.23}$$

---

* The exact values of $f(n) = a_{2n}^n$ are displayed in Table 5.1 in the next chapter.

Equating the terms independent of $1/n$ gives $S_p(x) = 0$ whose solution for $p = 1.25$ ($x_0 = 2.97710300694449$) has just been found. Exactly the same result is produced by equating the coefficients of $1/n$ on the two sides of (4.23). From the coefficients of $1/n^2$ however,

$$0 = c \sum_{t=1}^{\infty} \frac{x_0^t}{(2t)!} 2t\left(\frac{4p}{2t+2} - \frac{4}{2t+4}\right) - p x_0$$

$$= -2c\, x_0\, S_p'(x_0) - p x_0 \quad . \tag{4.24}$$

Taking $p = 1.25$, and obtaining the derivative $S_{1.25}'(x_0)$ from (4.18), we find $c = 1.631325858441925$. If required, this process can be continued (though with rapidly increasing labour) to give the numerical values of the constants involved in the terms of third and higher order.

Summarising, the solution for a_{2n}^n so far obtained is

$$a_{2n}^n = -.52715 \frac{(2n)!}{(2.97710300694449)^n}\left[1 + \frac{1.631325858441925}{2n} + O\left(\frac{1}{n^2}\right)\right]. \tag{4.25}$$

Chapter 5

NUMERICAL INVESTIGATION OF THE COEFFICIENTS a_ℓ^n AND OF THE ASSOCIATED POLYNOMIALS

In Chapter 4 it was shown that the recurrence relation (3.23) for a_ℓ^n simplified at the ends of the range for ℓ to permit an approximate solution for a_0^n and a_{2n}^n. Unfortunately (3.23) is much too complicated as it stands for similar results to be achieved for a_ℓ^n in general, and the next step is to seek an approximation to the R.H.S. of the equation which hopefully might make it more amenable to investigation and solution. This has been done here by direct numerical evaluation of the coefficients a_ℓ^n and concomitant inspection of which are the dominant contributions to the sum.

There are additional reasons why numerical analysis is appropriate at this stage:

(i) It is desirable to check the form of the solutions already found for a_0^n and a_{2n}^n, and to improve the numerical accuracy of the constant of proportionality in the expression for a_{2n}^n.

(ii) Eq. (4.9) predicts that a_0^n decreases steadily with n, while (4.25) forecasts a rapid increase for a_{2n}^n. Presumably, in the variation of a_ℓ^n with n, there is a value of ℓ at which there is a transition from dominance by a power to dominance by a factorial. It is therefore desirable to see, at least qualitatively, how a_ℓ^n varies with both n and ℓ.

(iii) When all the a_ℓ^n are known, it is a simple matter to calculate the values of the associated polynomials $\sum a^n_\ell x^\ell$ for different values of x. The existence of the $(2n)!$ factor in the numerator of the theoretical expression for a^n_{2n} suggests that the main series (3.7) in rising powers of y^2 may be asymptotic, i.e. that successive polynomials may increase in magnitude factorially, even after possible partial numerical cancellation of terms. This is obviously not the case for (at least) $x = 0$ however; it is therefore necessary to examine how the values of the polynomials vary with both x and n, and whether the main series (3.7) is hypergeometric or asymptotic. When this has been done, the worth of the series for the direct calculation of the function $\psi(x)$ may be estimated.

The numerical evaluation of a^n_ℓ from (3.23) by hand is only practicable up to about $n = 3$ or 4; beyond this, a digital computer must be brought into service. Here, an I.B.M. 1620 computer was programmed to calculate from (3.23) all the required coefficients and associated polynomials up to $n = 12$. Aspects of the computing problems encountered are discussed in Appendix 2. As in the previous chapter, p has been taken to be 1.25 throughout.

The resulting array of coefficients is displayed in Table 5.1. For computing purposes the indices ℓ and n are temporarily written as L and N respectively, and the number following "D" in the table is the power of 10 by which the listed value should be multiplied to give the value of a^n_ℓ .

5.1. Numerical Check on a^n_0 and a^n_{2n}

The theoretical result (4.9) for a^n_0 derived in the previous chapter implies that $(-\ a^{n-1}_0/a^n_0)$ should tend to 14.391169 as $n \to \infty$. Table 5.2 lists values of this quantity for n between 5 and12.

TABLE 5.1

THE a_L^N COEFFICIENTS UP TO N=12

(a_0^0 =1)

N= 1		N= 2	
L= 0	-0.555555555555555D-01	L= 0	0.378086419753086D-02
L= 1	0.666666666666666D 00	L= 1	0.398148148148148D 00
L= 2	-0.666666666666666D 00	L= 2	-0.239814814814815D 01
		L= 3	0.400000000000000D 01
		L= 4	-0.200000000000000D 01

N= 3		N= 4	
L= 0	-0.261855771115030D-03	L= 0	0.181835780151109D-04
L= 1	0.248858024691358D 00	L= 1	0.155000204128290D 00
L= 2	-0.540209876543210D 01	L= 2	-0.110449616238814D 02
L= 3	0.284842592592592D 02	L= 3	0.140869969135802D 03
L= 4	-0.596865740740740D 02	L= 4	-0.691458248456789D 03
L= 5	0.545333333333333D 02	L= 5	0.165046273148148D 04
L= 6	-0.181777777777778D 02	L= 6	-0.205887893518518D 04
		L= 7	0.129319259259259D 04
		L= 8	-0.323298148148148D 03

N= 5		N= 6	
L= 0	-0.126332890480001D-05	L= 0	0.877815112292487D-07
L= 1	0.965674350120324D-01	L= 1	0.601617501637262D-01
L= 2	-0.219771003563853D 02	L= 2	-0.433666774921737D 02
L= 3	0.616595334104062D 03	L= 3	0.256541353432640D 04
L= 4	-0.601391053218650D 04	L= 4	-0.461615891613371D 05
L= 5	0.282505639636610D 05	L= 5	0.381545053262119D 06
L= 6	-0.734037593399101D 05	L= 6	-0.174005176187918D 07
L= 7	0.111473632587448D 06	L= 7	0.479999502776549D 07
L= 8	-0.986530510040048D 05	L= 8	-0.836113373110030D 07
L= 9	0.471897619047619D 05	L= 9	0.926842640657332D 07
L=10	-0.943795238095237D 04	L=10	-0.634802170511536D 07
		L=11	0.245145623116402D 07
		L=12	-0.408576038527336D 06

N= 7

L= 0	-0.609961141504153D-08
L= 1	0.374809685380402D-01
L= 2	-0.853506221557465D 02
L= 3	0.104311843292588D 05
L= 4	-0.332874139252520D 06
L= 5	0.456764950899887D 07
L= 6	-0.337070435943662D 08
L= 7	0.150486407084395D 09
L= 8	-0.434025615149345D 09
L= 9	0.836936243577292D 09
L=10	-0.109107227848801D 10
L=11	0.950578543354474D 09
L=12	-0.530721711639678D 09
L=13	0.171827055883354D 09
L=14	-0.245467222690505D 08

N= 8

L= 0	0.423842684397205D-09
L= 1	0.233507652121383D-01
L= 2	-0.167841221006272D 03
L= 3	0.419555756826949D 05
L= 4	-0.232125646723021D 07
L= 5	0.511032485914575D 08
L= 6	-0.582534948066312D 09
L= 7	0.395693360300432D 10
L= 8	-0.173850450700695D 11
L= 9	0.518991365276004D 11
L=10	-0.108260899805473D 12
L=11	0.159672761649740D 12
L=12	-0.165954901052604D 12
L=13	0.118991242198339D 12
L=14	-0.560553150345169D 11
L=15	0.156226264596159D 11
L=16	-0.195282830745199D 10

N= 9

L= 0	-0.294515526294738D-10
L= 1	0.145476026354700D-01
L= 2	-0.329971959889566D 03
L= 3	0.167866919993372D 06
L= 4	-0.158864605128432D 08
L= 5	0.549217074678967D 09
L= 6	-0.939240630417977D 10
L= 7	0.934626266484204D 11
L= 8	-0.595871267821020D 12
L= 9	0.258547083373525D 13
L=10	-0.793334003167949D 13
L=11	0.176194684681226D 14
L=12	-0.286497017318669D 14
L=13	0.341305049598782D 14
L=14	-0.294614072770505D 14
L=15	0.179388881873920D 14
L=16	-0.730776092699128D 13
L=17	0.178778820125904D 13
L=18	-0.198643133473227D 12

N=10

L= 0	0.204650113978591D-11
L= 1	0.906320373691876D-02
L= 2	-0.648663516575251D 03
L= 3	0.669925689070226D 06
L= 4	-0.107563637383397D 09
L= 5	0.575819066465442D 10
L= 6	-0.144885446412141D 12
L= 7	0.205982791392290D 13
L= 8	-0.184673927548587D 14
L= 9	0.111985341697707D 15
L=10	-0.481054373093481D 15
L=11	0.150955784434933D 16
L=12	-0.352883503757698D 16
L=13	0.621145808658254D 16
L=14	-0.825523441348744D 16
L=15	0.823814971376252D 16
L=16	-0.607689863122006D 16
L=17	0.321449292638163D 16
L=18	-0.115336196719565D 16
L=19	0.251430343101024D 15
L=20	-0.251430343101024D 14

N=11

L= 0	-0.142205330662719D-12
L= 1	0.564640539250397D-02
L= 2	-0.127511838970833D 04
L= 3	0.267018336057155D 07
L= 4	-0.723748474306810D 09
L= 5	0.594353266270133D 11
L= 6	-0.217094149183816D 13
L= 7	0.433344966687060D 14
L= 8	-0.534655732648529D 15
L= 9	0.441273249102723D 16
L=10	-0.256928974122513D 17
L=11	0.109465395598825D 18
L=12	-0.349972775049437D 18
L=13	0.853779227678126D 18
L=14	-0.160509757006411D 19
L=15	0.233420627965509D 19
L=16	-0.261956544095479D 19
L=17	0.224742497628228D 19
L=18	-0.144678247570453D 19
L=19	0.676390030087061D 18
L=20	-0.216823188138930D 18
L=21	0.426240528943496D 17
L=22	-0.387491389948633D 16

N=12

L= 0	0.988142981312182D-14
L= 1	0.351772891600214D-02
L= 2	-0.250655901181916D 04
L= 3	0.106361913078389D 08
L= 4	-0.485191694907410D 10
L= 5	0.607370907573478D 12
L= 6	-0.318999635668414D 14
L= 7	0.882912420164143D 15
L= 8	-0.147594714530204D 17
L= 9	0.162706830396094D 18
L=10	-0.125537369831846D 19
L=11	0.706748667720161D 19
L=12	-0.299054191249490D 20
L=13	0.971300938613223D 20
L=14	-0.245666734929883D 21
L=15	0.488265191455337D 21
L=16	-0.765815950035890D 21
L=17	0.947429648056929D 21
L=18	-0.919343581768975D 21
L=19	0.691390165360424D 21
L=20	-0.394729111261921D 21
L=21	0.165314376139338D 21
L=22	-0.478870500077063D 20
L=23	0.857177487617625D 19
L=24	-0.714314573014688D 18

n	$-a_0^{n-1}/a_0^n$
5	14.3933840
6	14.3917424
7	14.3913284
8	14.3912155
9	14.3911830
10	14.3911734
11	14.3911704
12	14.3911694

Table 5.2

Evidently the approach to the limit is rapid, and application of any one of the standard techniques for accelerating the convergence of a sequence (e.g. the non-linear e_1- transform, see Shanks[32]) confirms that the limit in question is indeed 14.391169, correct to the last decimal digit quoted. Similarly, a list of $(-14.391169)^n a_0^n$ values shows that the multiplying constant in (4.9) is correctly taken to be 0.7797810.

The corresponding theoretical result (4.25)for a_{2n}^n likewise predicts the value 2.97710300694449 for the limit of the sequence $2n(2n-1)\, a_{2n-2}^{n-1} / a_{2n}^n$. Table 5.3 demonstrates that the approach to this limit is extremely slow, and here the e_1 transform proves

n	$2n(2n-1)\, a_{2n-2}^{n-1} / a_{2n}^n$
5	3.0829 60387 89688
6	3.0491 50211 49083
7	3.0293 59203 11171
8	3.0167 59498 05276
9	3.0082 36185 32402
10	3.0021 98930 67945
11	2.9977 65151 06753
12	2.9944 12480 60954

Table 5.3

comparatively ineffective as an accelerator of convergence. This is because successive terms in the sequence vary approximately linearly with $1/n$, and the e_1 transform operating on any sequence of the form

$$a_n = a + \frac{b}{n} + O\left(\frac{1}{n^2}\right) \tag{5.1}$$

yields

$$e_1(a_n) = a + \frac{b}{2n} + O\left(\frac{1}{n^2}\right). \tag{5.2}$$

Probably the most efficient technique for determining the limit of a sequence of this type is Salzer's modification[47] of the well known Lagrange interpolation formula. This extrapolates to $1/n = 0$ the known sequence values fitted to polynomials in the variable $1/n$. For the figures in Table 5.3, the 4-point formula based on $n = 12$ (i.e. utilising the sequence values from $n = 9$ to $n = 12$) predicts the limit 2.97687, while the more accurate 7-point formula * (utilising the values from $n = 6$ to $n = 12$) yields 2.97709. This adequately confirms the theoretical value, and provides a guide as to how accurately the sequence limit may be estimated from the numbers produced by such formulae, in later applications where the theoretical limit is not already known.

To verify the value of the constant in the second order term in the expression for a^n_{2n}, we first note that (4.25) implies

$$2n^2\left[1 - \frac{a^n_{2n}\; 2.97710300694449}{a^{n-1}_{2n-2}\; 2n(2n-1)}\right] = 1.631325858441925 + O\left(\frac{1}{n}\right). \tag{5.3}$$

---

* To obtain full accuracy with the 7-point formula, the sequence values must be known to approximately (k + 8) significant figures, where k is the number of significant figures required in the limit. This is why many of the "raw" numerical values have been quoted to up to 15 decimal digits.

Successive values of the L.H.S. have been evaluated, whose limit estimated by the 7-point Salzer formula agrees to five significant figures with the theoretical value on the R.H.S.

The constant of proportionality in (4.25) is on a different footing from the other constants dealt with so far, because approximations were introduced in its evaluation and the resulting error is difficult to estimate. The best way to find an accurate value for this constant is to calculate successive values of

$$a_{2n}^{n}\ \frac{(2.97710300694449)^{n}}{(2n)!}\left[1+\frac{1.631325858441925}{2n}\right]^{-1} \qquad (5.4)$$

and extrapolate to $1/n = 0$. Table 5.4 exhibits the sequence values obtained by this procedure, and the 4-point and 7-point Salzer

n	Estimate of proportionality const.
5	−0.52294 35766 24191
6	−0.52280 80231 04123
7	−0.52272 63650 44587
8	−0.52267 33653 42369
9	−0.52263 70124 49697
10	−0.52261 09931 58134
11	−0.52259 17286 58208
12	−0.52257 70663 74184

Table 5.4

formulae applied to these predict limits of −0.522499260 and −0.522499791 respectively. We may safely conclude therefore that a more accurate version of (4.25) is

$$a^{n}_{2n} = -.522499 \frac{(2n)!}{(2.977103006944449)^{n}} \left[1 + \frac{1.631325858441925}{2n} + O\left(\tfrac{1}{n^2}\right) \right] \quad (5.5)$$

5.2. Numerical Inspection of the Coefficients a^{n}_{ℓ}

When calculating the numerical values of a^{n}_{ℓ} by hand for small n , it was noted that by far the greatest contribution to a^{n}_{ℓ} in the t-summation in (3.23) is that for which $t=1$. For instance, the value of a^{3}_{4} is -59.686, the contribution from $t=1$ being -49.285. As n increases, the $t=1$ contribution becomes increasingly dominant, so that a^{n}_{ℓ} is determined to an ever-increasing extent by the a^{n-1}_{s} coefficients alone. This observation is the basis of an approximation to a^{n}_{ℓ} [and correspondingly to $\psi(x)$] which is derived and discussed in Chapter 7.

Inspection of Table 5.1 reveals the general tendency for the a^{n}_{ℓ} coefficients to increase rapidly in magnitude with n, reaching values up to $\simeq 10^{21}$ for $n=12$. For $\ell = 0$ and $\ell = 1$ the coefficients decrease, somewhat slowly in the latter case; at $\ell = 2$ they slowly increase with n, and thereafter the increase becomes more rapid. There is a fairly sharp, asymmetrical peak in a^{n}_{ℓ} for fixed n and varying ℓ , the maximum occurring at about $\ell = 3/2$ n.

It is interesting to note that $(-1)^{\ell} a^{n}_{\ell} / a^{n}_{2n}$ is roughly equal to the binomial coefficient $\binom{n}{2n-\ell}$, at least for $\ell \gtrsim n$, as is illustrated in Table 5.5 for $n=7$. This serves as the basis for an approximate, empirical solution for a^{n}_{ℓ} which will be discussed further in Chapter 7. It will be shown there that such an approximation is unfortunately inadequate for further application. Essentially this is because there is a high degree of cancellation

ℓ	$(-1)^{\ell} a_{\ell}^{7} / a_{14}^{7}$	$\binom{7}{14-\ell}$
0	0.000	
1	0.000	
2	0.000	
3	0.000	
4	0.014	
5	0.186	
6	1.373	
7	6.131	1
8	17.682	7
9	34.096	21
10	44.449	35
11	38.725	35
12	21.621	21
13	7.000	7
14	1.000	1

Table 5.5

of contributions if the polynomials $\sum a_{\ell}^{n} x^{\ell}$ (see next section), so that any error in the estimate of the individual coefficients causes a large error in the estimate of the sum.

5.3 Numerical Evaluation of the Associated Polynomials

Table 5.6 lists values of the polynomial $\sum a_{\ell}^{n} x^{\ell}$ for n = 7 and values of x in the range 0 to 0.5. [Since $\phi(\eta) = \phi(-\eta)$, (3.5) and (3.6) imply that $\psi(x) = \psi(1-x)$. There is no need therefore to cover also the range 0.5 to 1, other than as a check for possible computational errors.]

x	$\sum_{\ell=0}^{14} a_\ell^7 x^\ell$
0.00	-6.0996×10^{-9}
0.05	0.01480
0.10	-0.29133
0.15	0.20826
0.20	1.17812
0.25	0.56707
0.30	-1.56052
0.35	-2.69727
0.40	-1.10573
0.45	1.94922
0.50	3.47973

Table 5.6

Comparing with Table 5.1, it will be observed that the values of the polynomial are generally several orders of magnitude smaller than the corresponding coefficients, indicating almost complete cancellation of contributions. This feature is found for all other large values of n.

More detailed evaluation of the polynomial for intermediate values of x reveals an oscillatory pattern of behaviour, the reason for the variation in sign of the numbers in Table 5.6. The amplitude of the oscillation is largest for $x = 0.5$ and decreases with increasing rapidity as x decreases, becoming extremely small near $x = 0$. At the same time the period of the oscillation increases, so that the majority of the zeros of the polynomial are nearer $x = 0$ than $x=0.5$. For $n = 7$, $\sum a_\ell^n x^\ell$ has 7 zeros in the range $0 < x < 0.5$. (The other 7 obviously lie in the range $0.5 < x < 1$). In general the n'th polynomial has n zeros in this range if n is odd, and $(n-1)$ zeros if n is even, an additional zero lying just to the left of the origin.

Considering now the variation with n, the general tendency is for the magnitude of the n'th polynomial to increase with n after an initial decrease, in accordance with the conjectured factorial behaviour. Table 5.7 below illustrates this for $x = 0.5$. In Chapter 8 it will be shown that the n'th polynomial contains a multiplying factor $(2n)!$, confirming the generally asymptotic nature of the series (3.7). The point $x = 0$ (and correspondingly $x = 1$) is exceptional in this respect; at this point, the polynomial reduces to the single term a_0^n whose form is given by (4.9).

n	$\sum_{\ell=0}^{2n} a_\ell^n (.5)^\ell$
0	1.0000
1	1.1111×10^{-1}
2	-2.1682×10^{-2}
3	2.3903×10^{-2}
4	-4.3956×10^{-2}
5	1.3043×10^{-1}
6	-5.7208×10^{-1}
7	3.4797
8	-2.8022×10^{1}
9	2.8854×10^{2}
10	-3.6971×10^{3}
11	5.7684×10^{4}
12	-1.0766×10^{6}

Table 5.7

We may now note the rather limited utility of the series (3.7) for numerical estimation of the function ψ, if it were simply to be broken off at the least term and the remainder discarded. For $x = 0.5$, the coefficients of y^{2n} are the numbers in Table 5.7. Now the error in the estimate of a function, retaining that part of its asymptotic expansion for which successive terms decrease, is of the order of the last term included in the summation. If our criterion of utility is that the estimate shall be within 1% of the exact value of the function, it will be seen from the above table that this is achieved only in the high temperature region $y \lesssim 1$. This conclusion is unchanged for other values of x in the range $0 < x < 1$.

Chapter 6

TRANSFORMATION TO A MORE SUITABLE INDEPENDENT VARIABLE

There are a number of reasons why we must now revise our original choice of x as the independent variable.

Firstly, the coefficients a_ℓ^n are not all independent. As pointed out in § 5.3, the fact that $\phi(\eta)$ is an even function of η implies that $\psi(x) = \psi(1-x)$, so that

$$\sum_{\ell=0}^{2n} a_\ell^n x^\ell = \sum_{\ell=0}^{2n} a_\ell^n (1-x)^\ell . \qquad (6.1)$$

Expanding the R.H.S. in rising powers of x and equating coefficients of equal powers of x on the two sides,

$$a_\ell^n = (-1)^\ell \sum_{s=\ell}^{2n} a_s^n \binom{s}{\ell} . \qquad (6.2)$$

For fixed n, there are n non-trivial equations of this type so that only (n+1) of the (2n+1) coefficients a_ℓ^n are independent. We therefore have to enquire whether a better choice of variable could not be made for which the corresponding polynomial would have only (n+1) independent coefficients.

Secondly, the coefficients a_ℓ^n are typically many orders of magnitude greater than the polynomials to which they contribute. For such mighty contributions to sum to such a (comparatively) puny answer smacks of inefficiency, not to mention the computing difficulties when there is such wholesale cancellation of terms; and one would hope that the coefficients associated with any new variable would be considerably smaller in magnitude.

Thirdly the origin $x = 0$ is an atypical point in the range $0 \leqslant x \leqslant 1$. Whereas the general tendency is for the n'th polynomial to increase with n through the eventual dominance of the $(2n)!$ factor, only at $x = 0$ (and, of course, at $x = 1$) does it consistently decrease. This reflects the peculiarity of the coefficient a_0^n and suggests that the determination of the form of a_0^n in Chapter 4 is unfortunately not likely to be of great significance in the eventual calculation of the function ψ. Hopefully, the two extremities of any new set of coefficients should not only be conducive to analysis but also of benefit to the calculation of ψ.

All these expected benefits may be realised, although accompanied by one drawback, if we choose as a new independent variable the quantity

$$X = 1 - 2x = \frac{e^{\eta} - 1}{e^{\eta} + 1} . \qquad (6.3)$$

Clearly the physically interesting range for X is $-1 \leqslant X \leqslant 1$. Writing

$$\psi(x) = \Psi(X) , \qquad (6.4)$$

it is evident that Ψ is an even function of X, so that only even powers of X can appear in the various polynomials which arise. Correspondingly, it will be sufficient to investigate only the region $0 \leqslant X \leqslant 1$, and the integral in (3.8) which we must finally evaluate is, in terms of the new variable,

$$\frac{1}{2} \int_{-1}^{1} \Psi(X)\, dX = \int_{0}^{1} \Psi(X)\, dX . \qquad (6.5)$$

In comparison with (3.7), our expectation is that the equivalent expansion of Ψ will be

$$\Psi(X) = \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{r} A_s^r \, X^{2s}, \tag{6.6}$$

and we must now substitute this into the integral equation to find the recurrence relation for the coefficients A_s^r.

6.1. Recurrence Relation for the Coefficients A_s^r

The derivation of the recurrence relation for A_s^r is similar to but somewhat more complicated than that for a_s^r. We begin by expressing the integral equation (3.9) in terms of the new function Ψ :

$$\frac{1}{4} y^4 = \int_{-y}^{y} \frac{dz \, z^2}{[(1-X)+e^{z}(1+X)]/|1-e^{-z}|} \left\{ p y^2 \, \Psi(X) - (p y^2 - z^2)\, \Psi\left[\frac{(1+X)e^{z}-(1-X)}{(1+X)e^{z}+(1-X)}\right] \right\}. \tag{6.7}$$

Expanding Ψ (X) in accordance with (6.6),

$$\frac{1}{4} y^4 = \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{r} A_s^r \int_{-y}^{y} \frac{dz\, z^2}{|z|}\left(\frac{-z}{e^{-z}-1}\right)\left\{\frac{p y^2 X^{2s}}{(1+X)e^{z}+(1-X)} - (p y^2 - z^2)\frac{[(1+X)e^{z}-(1-X)]^{2s}}{[(1+X)e^{z}+(1-X)]^{2s+1}}\right\}. \tag{6.8}$$

Recalling that (3.12) provides a recipe for the expansion of any function of e^{z} in rising powers of z,

$$\frac{[(1+X)e^{z}-(1-X)]^{2s}}{[(1+X)e^{z}+(1-X)]^{2s+1}} = \frac{1}{2} \sum_{m=0}^{\infty} \frac{z^m}{m!} \sum_{\nu=0}^{m} C_m^{\nu} \, \nu! \left(-\tfrac{1}{2}\right)^{\nu} (1+X)^{\nu} \sum_{n=0}^{2s,\nu} (-1)^n \binom{\nu}{n} \binom{2s+\nu-n}{\nu} X^{2s-n}. \tag{6.9}$$

Combining this with (3.11) and taking advantage of (3.15),

$$\left(\frac{-z}{e^{-z}-1}\right)\frac{\left[(1+X)e^{z}-(1-X)\right]^{2s}}{\left[(1+X)e^{z}+(1-X)\right]^{2s+1}} = \frac{1}{2}\sum_{\ell=0}^{\infty}\frac{z^{\ell}}{\ell!}(-1)^{\ell}\sum_{m=0}^{\ell}\binom{\ell}{m}(-1)^{m}B_{\ell-m}\sum_{\nu=0}^{m}C^{\nu}_{m}\,\nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}$$

$$\times\sum_{n=0}^{2s,\nu}(-1)^{n}\binom{\nu}{n}\binom{2s+\nu-n}{\nu}X^{2s-n}$$

$$= \frac{1}{2}\sum_{\ell=0}^{\infty}\frac{z^{\ell}}{\ell!}(-1)^{\ell}\sum_{\nu=0}^{\ell}\nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\sum_{n=0}^{2s,\nu}(-1)^{n}\binom{\nu}{n}\binom{2s+\nu-n}{\nu}X^{2s-n}$$

$$\times\sum_{m=0}^{\ell}\binom{\ell}{m}(-1)^{m}B_{\ell-m}\,C^{\nu}_{m}$$

$$= \frac{1}{2}\sum_{\ell=0}^{\infty}\frac{z^{\ell}}{\ell!}\sum_{\nu=0}^{\ell}\nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\frac{\ell}{\nu}C^{\nu}_{\ell}\sum_{n=0}^{2s,\nu}(-1)^{n}\binom{\nu}{n}\binom{2s+\nu-n}{\nu}X^{2s-n}.$$

$$(6.10)$$

On substitution, (6.8) becomes

$$\frac{1}{4}y^{4} = \frac{1}{2}\sum_{r=0}^{\infty}y^{2r}\sum_{s=0}^{r}A^{r}_{s}X^{2s}\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\sum_{\nu=0}^{\ell}\nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\frac{\ell}{\nu}C^{\nu}_{\ell}\int_{-y}^{y}\frac{dz\,z^{\ell+2}}{|z|}$$

$$\times\left\{\rho y^{2}-(\rho y^{2}-z^{2})\sum_{n=0}^{2s,\nu}(-1)^{n}\binom{\nu}{n}\binom{2s+\nu-n}{\nu}X^{-n}\right\}$$

$$= \sum_{r=0}^{\infty}y^{2r}\sum_{s=0}^{r}A^{r}_{s}X^{2s}\sum_{\ell=0,2,4\ldots}^{\infty}\frac{1}{\ell!}\sum_{\nu=0}^{\ell}\nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\frac{\ell}{\nu}C^{\nu}_{\ell}$$

$$\times\left\{\frac{\rho y^{\ell+4}}{\ell+2}-\left(\frac{\rho y^{\ell+4}}{\ell+2}-\frac{y^{\ell+4}}{\ell+4}\right)\sum_{n=0}^{2s,\nu}(-1)^{n}\binom{\nu}{n}\binom{2s+\nu-n}{\nu}X^{-n}\right\}$$

$$= \frac{1}{4} y^4 \sum_{r=0}^{\infty} y^{2r} \sum_{s=0}^{r} A_s^r X^{2s} \sum_{t=0}^{\infty} \frac{y^{2t}}{(2t)!} \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu}$$

$$\times \left\{ \frac{4\rho}{2t+2} - \left(\frac{4\rho}{2t+2} - \frac{4}{2t+4} \right) \sum_{n=0}^{2s,\nu} (-1)^n \binom{\nu}{n} \binom{2s+\nu-n}{\nu} X^{-n} \right\}$$

$$= \frac{1}{4} y^4 \sum_{n=0}^{\infty} y^{2n} \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu}$$

$$\times \left\{ \frac{4\rho}{2t+2} - \left(\frac{4\rho}{2t+2} - \frac{4}{2t+4} \right) \sum_{m=0}^{2s,\nu} (-1)^m \binom{\nu}{m} \binom{2s+\nu-m}{\nu} X^{-m} \right\}. \tag{6.11}$$

Equating coefficients of powers of y ,

$$A_0^0 = 1 \tag{6.12}$$

and, for $n = 1, 2 \ldots \infty$,

$$0 = \sum_{t=0}^{n} \frac{1}{(2t)!} \sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu}$$

$$\times \left\{ \frac{4\rho}{2t+2} - \left(\frac{4\rho}{2t+2} - \frac{4}{2t+4} \right) \sum_{m=0}^{2s,\nu} (-1)^m \binom{\nu}{m} \binom{2s+\nu-m}{\nu} X^{-m} \right\}. \tag{6.13}$$

Now

$$\sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} = \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \sum_{q=0}^{\nu} \binom{\nu}{q} X^q \frac{2t}{\nu} C_{2t}^{\nu}$$

$$= \sum_{q=0}^{2t} X^q \sum_{\nu=q}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \binom{\nu}{q}. \tag{6.14}$$

It is shown in Appendix 1 that the final summation over ν is zero if q is odd. This also follows from the easily demonstrated fact that the R.H.S. of (6.8) is an even function of X, so that only even powers of X can be involved. Hence

$$\sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\ \tfrac{2t}{\nu}\ C_{2t}^{\nu} =$$

$$= \sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{r=0}^{t} X^{2r} \sum_{\nu=2r}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \tfrac{2t}{\nu}\ C_{2t}^{\nu}\binom{\nu}{2r}$$

$$= \sum_{\ell=0}^{n} X^{2\ell} \sum_{r=0,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=2r}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \tfrac{2t}{\nu}\ C_{2t}^{\nu}\binom{\nu}{2r}. \tag{6.15}$$

Similarly,

$$\sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu}\ \tfrac{2t}{\nu}\ C_{2t}^{\nu} \sum_{m=0}^{2s,\nu}(-1)^m\binom{\nu}{m}\binom{2s+\nu-m}{\nu} X^{-m} =$$

$$= \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \tfrac{2t}{\nu}\ C_{2t}^{\nu} \sum_{\ell=0}^{\nu}\binom{\nu}{\ell}X^{\ell} \sum_{m=0}^{2s,\nu}(-1)^m\binom{\nu}{m}\binom{2s+\nu-m}{\nu} X^{-m}$$

$$= \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \tfrac{2t}{\nu}\ C_{2t}^{\nu} \sum_{q=-2s,-\nu}^{\nu} X^{q} \sum_{m=0,-q}^{2s,\nu,\nu-q}(-1)^m\binom{\nu}{m+q}\binom{\nu}{m}\binom{2s+\nu-m}{\nu}$$

$$= \sum_{q=-2s,-2t}^{2t} X^{q} \sum_{\nu=|q|}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \tfrac{2t}{\nu}\ C_{2t}^{\nu} \sum_{m=0,-q}^{2s,\nu,\nu-q}(-1)^m\binom{\nu}{m+q}\binom{\nu}{m}\binom{2s+\nu-m}{\nu}. \tag{6.16}$$

The double summation over ν and m must be zero if q is odd, since the R.H.S. of (6.8)is even in X and so only even powers of X can be involved. Hence

$$\sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{\nu=0}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu}(1+X)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \sum_{m=0}^{2s,\nu} (-1)^m \binom{\nu}{m}\binom{2s+\nu-m}{\nu} X^{-m} =$$

$$= \sum_{s=0}^{n-t} A_s^{n-t} X^{2s} \sum_{r=-s,-t}^{t} X^{2r} \sum_{\nu=|2r|}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \sum_{m=0,-2r}^{2s,\nu,\nu-2r} (-1)^m \binom{\nu}{m+2r}\binom{\nu}{m}\binom{2s+\nu-m}{\nu}$$

$$= \sum_{\ell=0}^{n} X^{2\ell} \sum_{r=-t,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=|2r|}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \sum_{m=0,-2r}^{2\ell-2r,\nu,\nu-2r} (-1)^m \binom{\nu}{m+2r}\binom{\nu}{m}\binom{2\ell-2r+\nu-m}{\nu}.$$

(6.17)

Combining (6.13), (6.15) and (6.17), and equating to zero the coefficient of $X^{2\ell}$ in the range $0 \leqslant \ell \leqslant n$,

$$0 = \sum_{t=0}^{n} \frac{1}{(2t)!} \left\{ \frac{4P}{2t+2} \sum_{r=0,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=2r}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \binom{\nu}{2r} \right.$$

$$\left. - \left(\frac{4P}{2t+2} - \frac{4}{2t+4}\right) \sum_{r=-t,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=|2r|}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \sum_{m=0,-2r}^{2\ell-2r,\nu,\nu-2r} (-1)^m \binom{\nu}{m+2r}\binom{\nu}{m}\binom{2\ell-2r+\nu-m}{\nu} \right\}.$$

(6.18)

It follows that the recurrence relation is

$$A_\ell^n = \sum_{t=1}^{n} \frac{1}{(2t)!} \left(\frac{4P}{2t+2} - \frac{4}{2t+4}\right) \sum_{r=-t,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=|2r|}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} C_{2t}^{\nu} \sum_{m=0,-2r}^{2\ell-2r,\nu,\nu-2r} (-1)^m \binom{\nu}{m+2r}\binom{\nu}{m}\binom{2\ell-2r+\nu-m}{\nu}$$

$$- \sum_{t=1}^{n} \frac{1}{(2t)!} \frac{4P}{2t+2} \sum_{r=0,\ell-n+t}^{t,\ell} A_{\ell-r}^{n-t} \sum_{\nu=2r}^{2t} \nu!\left(-\tfrac{1}{2}\right)^{\nu} \frac{2t}{\nu} \cdot C_{2t}^{\nu} \binom{\nu}{2r}.$$

(6.19)

It does not appear possible to express the remaining summations over ν in more concise form (see Appendix 1) and (6.19) is therefore believed to be the simplest generator of the coefficients A_ℓ^n starting from $A_0^0 = 1$.

6.2. Discussion of the New Coefficients A_ℓ^n

The recurrence relation (6.19) is more complicated than (3.23) for a_ℓ^n, there being one additional summation to carry out. The two sets of coefficients are related through the requirement

$$\sum_{\ell=0}^{n} A_\ell^n X^{2\ell} = \sum_{\ell=0}^{2n} a_\ell^n x^\ell . \tag{6.20}$$

Since $x = \frac{1}{2}(1-X)$, we may expand the R.H.S. in rising powers of X which yields, on equating coefficients of the even powers of X,

$$A_\ell^n = \sum_{m=2\ell}^{2n} a_m^n \left(\tfrac{1}{2}\right)^m \binom{m}{2\ell} . \tag{6.21}$$

In particular,

$$A_n^n = a_{2n}^n \left(\tfrac{1}{2}\right)^{2n} . \tag{6.22}$$

Using the previously derived values for a_ℓ^n, these equations serve as a numerical check on the values of A_ℓ^n calculated from (6.19).

Putting $\ell = n$ in (6.19), the recurrence equation for A_n^n reduces to a form very similar to (4.12) for a_{2n}^n. This is just as expected of course, through (6.22). We deduce from (5.5) and (6.22) that

$$A_n^n \simeq -.522499 \frac{(2n)!}{(11.908412027777\,96)^n}\left[1 + \frac{1.631325858441925}{2n} + O\left(\frac{1}{n^2}\right)\right]. \tag{6.23}$$

Unfortunately there is no equally drastic simplification in (6.19) on putting $\ell = 0$; the coefficients A_o^n do <u>not</u> depend on the lower order coefficients A_o^s alone. Consequently it is no easier to find an approximate solution for A_o^n than it is to solve for A_ℓ^n in general. It will be shown by numerical analysis in Chapter 8, however, that in spite of the complexity of the recurrence relation, the approximate form of A_o^n for large n is the same as (6.23) but with different numerical values of the constants.

An IBM 360 computer has been programmed to calculate the coefficients A_ℓ^n from the recurrence relation (6.19) together with the associated polynomials $\sum A_\ell^n X^{2\ell}$ from $n = 1$ to 20, starting from $A_o^o = 1$. Again, p has been taken to be 1.25 . As with the previous coefficients, the A_ℓ^n increase quite rapidly with n, but not nearly so fast as the a_ℓ^n . When $n = 10$ for example, the maximum of the range A_ℓ^n ($\ell = 0,1\ldots n$) is $\sim 10^8$,compared with $\sim 10^{15}$ for a_ℓ^n. It follows that the extent of numerical cancellation of contributions on the L.H.S. of (6.20) is nowhere near so great as occurs in the R.H.S.

Unlike the other coefficients, there are no values of ℓ for which A_ℓ^n decreases with increasing n. However there is again a fairly sharp asymmetrical peak in A_ℓ^n for fixed n but varying ℓ , the maximum occurring this time at about $\ell = \frac{2}{3}n$. This is illustrated by Table 6.1 which lists the coefficients A_ℓ^7 , $\ell = 0,1\ldots7$.

ℓ	A_ℓ^7
0	3.4797×10^0
1	-1.6802×10^2
2	1.5555×10^3
3	-5.9704×10^3
4	1.1699×10^4
5	1.2388×10^4
6	6.7666×10^3
7	1.4982×10^3

<u>Table 6.1</u>

Summarising, selection of the new independent variable X has resulted in fewer, independent coefficients in our trial expansion of the function Ψ . These new coefficients are, on the whole, smaller in magnitude than the old ones, and give rise to lesser computational problems associated with the almost complete cancellation of very large terms. There is every reason to believe that $X = 0$ – the new origin – is a typical point in the physical range of interest $(0 \leqslant X \leqslant 1)$. (In Chapter 8 it will be shown that $X = 0$ is indeed a specially important point). All this is achieved at the expense of a rather more complicated recurrence relation (6.19) than we had previously; for purely numerical work, this is immaterial.

Chapter 7

AN APPROXIMATE SOLUTION $\hat{\Psi}(x)$ IN CLOSED FORM, VALID AT MODERATE AND HIGH TEMPERATURES.

In §5.2 we noted that the dominant contribution to a_ℓ^n in the summation over t on the R.H.S. of (3.23) is that for which t = 1; the extent of this dominance increases with n. Exactly the same is true for the A_ℓ^n coefficients generated by (6.19), as might have been predicted from (6.21). [For convenience, most of this discussion is in terms of the original variable x with corresponding coefficients a_ℓ^n ; equivalent conclusions are just as easily reached when based on the corresponding quantities X and A_ℓ^n].

This observation suggests that yet another set of coefficients, analogous to a_ℓ^n and denoted by $\hat{a}_\ell^n$, may conveniently be defined, the definition being the same as (3.23) except that only the first term in the t-summation is retained. Thus

$$\hat{a}_\ell^n = \sum_{\gamma=0,\ell-2n+2}^{2,\ell} \hat{a}_{\ell-\gamma}^{n-1} (-1)^\gamma \left\{ \left(p-\tfrac{2}{3}\right)\binom{\ell}{\gamma} \sum_{\nu=\gamma}^{2,\ell} \frac{\nu!}{2} \, \frac{2}{\nu} \, C_2^\nu \binom{\ell-\gamma}{\nu-\gamma} - p\,\frac{\gamma!}{2}\,\frac{2}{\gamma}\,C_2^\gamma \right\}, \tag{7.1}$$

with $\hat{a}_0^0 = 1$. If ℓ is not equal to 0,1,2n or 2n-1, this may be written as

$$\hat{a}_\ell^n = -\tfrac{1}{18}\hat{a}_\ell^{n-1} + \tfrac{2}{3}\hat{a}_{\ell-1}^{n-1} - \tfrac{2}{3}\hat{a}_{\ell-2}^{n-1} + \mu(\ell+1)\left[\ell\,\hat{a}_\ell^{n-1} - 2(\ell-1)\hat{a}_{\ell-1}^{n-1} + (\ell-2)\hat{a}_{\ell-2}^{n-1}\right] \tag{7.2}$$

where

$$\mu = \tfrac{1}{2}\left(p - \tfrac{2}{3}\right). \tag{7.3}$$

When ℓ does assume one of these special values, the only terms in the expression for $\hat{a}_\ell^n$ which are retained are those on the R.H.S. of (7.2) for which the lower suffix of $\hat{a}$ lies in the allowed range $0 \leqslant$ suffix $\leqslant 2n-2$. To avoid having to write each of these special cases separately, it is convenient to allow ℓ in $\hat{a}_\ell^n$ to assume all integer values from $-\infty$ to $+\infty$ and define

$$\hat{a}_m^0 = \begin{cases} 1, & m = 0 \\ 0, & m \neq 0 \end{cases} . \tag{7.4}$$

Successive applications of (7.2) for n = 1,2... then yield the correct values for $\hat{a}_\ell^n$ when $0 \leqslant \ell \leqslant 2n$ and zero when ℓ lies outside this range.

From the manner of their definition, we expect that the coefficients $\hat{a}_\ell^n$ will be approximations, in some sense, to the original coefficients a_ℓ^n. This is borne out by computer evaluation of $\hat{a}_\ell^n$ by (7.2) with p = 1.25: $\hat{a}_\ell^n$ matches a_ℓ^n very closely in its variation with n and ℓ although it is generally smaller in magnitude, the difference increasing with n. In § 5.2 we remarked that a_ℓ^n was roughly equal to $(-1)^\ell \binom{n}{2n-\ell} a_{2n}^n$, at least for $\ell \gtrsim n$. A corresponding relation is observed numerically for $\hat{a}_\ell^n$ so, combining the two, we get

$$\frac{\hat{a}_\ell^n}{\hat{a}_{2n}^n} \cdot \frac{a_{2n}^n}{a_\ell^n} \simeq 1 . \tag{7.5}$$

To illustrate how closely this approximate equation is satisfied, Table 7.1 lists values of the L.H.S. for n = 7 and ℓ = 0,1....14. As n increases, the corresponding values steadily approach 1 for all values of ℓ except ℓ = 0 and ℓ = 1.

Corresponding to the new coefficients $\hat{a}_\ell^n$, we define, in analogy with (3.7), a new function

$$\hat{\psi}(x) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell , \tag{7.6}$$

ℓ	$\frac{\hat{a}_\ell^7}{\hat{a}_{14}^7} \cdot \frac{a_{14}^7}{a_\ell^7}$
0	0.80252
1	1.04233
2	1.03414
3	1.02136
4	1.01344
5	1.00857
6	1.00547
7	1.00344
8	1.00210
9	1.00122
10	1.00064
11	1.00028
12	1.00008
13	1.00000
14	1.00000

Table 7.1

and we shall investigate the circumstances under which this is an approximation to the original function ψ. Numerically, the polynomials $\sum \hat{a}_\ell^n x^\ell$ show the same variation with x and n as the polynomials $\sum a_\ell^n x^\ell$ discussed in § 5.3, but are generally slightly smaller in magnitude. In view of (7.5), it is tempting to assume

$$\frac{\sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell}{\sum_{\ell=0}^{2n} a_\ell^n x^\ell} \cdot \frac{a_{2n}^n}{\hat{a}_{2n}^n} \simeq 1 . \tag{7.7}$$

Table 7.2 shows calculated values of the L.H.S. for n = 7, demonstrating the essential correctness of this surmise. (This is somewhat surprising, in view of the large-scale cancellation occurring in each summation.) As n increases, the corresponding values tend

x	L.H.S. of (7.7) for n = 7
0	0.8025
0.1	1.0090
0.2	0.9985
0.3	0.9645
0.4	0.9976
0.5	0.9766

Table 7.2

to approach 1, but do not do so uniformly. This is due to the oscillatory variation of the polynomials with x; atypical values of the L.H.S. of (7.7) occur when by chance the value of x we select lies close to a zero of either polynomial.

There are at least two methods by which a more or less exact solution for $\hat{\psi}$ might conceivably be obtained. The first is to find a reasonably accurate solution of (7.2) and then to carry out the double summation in (7.6). The second involves demonstrating that $\hat{\psi}(x)$ is the solution of an inhomogeneous differential equation of second order. The first method proves far inferior to the second, but it will nevertheless be briefly discussed to emphasize the difficulties and dangers when there is widespread cancellation of terms as there is in (7.6).

7.1 First Method: Approximate Solution for $\hat{a}_\ell^n$ and Reasons for Rejection.

Any approximation to $\hat{a}_\ell^n$ is likely to be most accurate at one or other of the ends of the range for ℓ , viz. $\ell = 0$ and $\ell = 2n$, and to be progressively more in error as ℓ moves away from these values. These end-points for ℓ are the only two values in the neighbourhood of which (7.2) simplifies sufficiently for a solution to be readily calculable, e.g. :

$$\ell = 0 : \quad \hat{a}_0^n = \left(-\tfrac{1}{18}\right) \hat{a}_0^{n-1} . \tag{7.8}$$

$$\begin{aligned} \ell = 2n : \quad \hat{a}_{2n}^n &= \left[-\tfrac{2}{3} + \mu (2n+1)(2n-2) \right] \hat{a}_{2n-2}^{n-1} \\ &= 4\mu (n+\xi)(n-\xi-\tfrac{1}{2})\, \hat{a}_{2n-2}^{n-1} , \end{aligned} \tag{7.9}$$

where

$$\xi(\xi + \tfrac{1}{2}) = \tfrac{1}{2} + \frac{1}{6\mu} = \frac{P}{4\mu} . \tag{7.10}$$

The solutions are therefore

$$\hat{a}_0^n = \left(-\tfrac{1}{18}\right)^n , \tag{7.11}$$

$$\hat{a}_{2n}^n = (4\mu)^n \frac{(n+\xi)!\,(n-\xi-\frac{1}{2})!}{\xi!\,(-\xi-\frac{1}{2})!} . \tag{7.12}$$

The difficulty with $\ell = 0$ as an end-point on which to base an approximation for $\hat{a}_\ell^n$ is that $\hat{a}_0^n$ (like a_0^n) is completely atypical in its variation with n (e.g. decreasing instead of increasing as n increases through large values.) As the value of the polynomial $\sum \hat{a}_\ell^n x^\ell$ at x = 0, it bears no comparison with the average magnitude of the same polynomial for small but non-zero values of x. Accurate knowledge of $\hat{a}_\ell^n$ near $\ell = 0$ only matters therefore when calculating the polynomials in the unimportant range of vanishingly small x; outside this range the higher coefficients are quickly dominant, and they are very unlikely to be predicted accurately by any approximation which is most accurate at $\ell = 0$.

The other end point $\ell = 2n$ is hardly much better. Given an approximation for $\hat{a}^n_\ell$ which is most accurate for $\ell \simeq 2n$, only in the 'non-physical' region $x >> 1$ do the contributions of the accurately known coefficients dominate in the evaluation of the n'th polynomial, so only there is the value of the latter likely to be predicted with small error. In the 'physical' region $0 \leqslant x \leqslant 1$, the contribution associated with <u>every</u> coefficient $\hat{a}^n_\ell$ is important, since together they almost completely cancel each other out. Any inaccuracy in the estimate of any of these coefficients is likely to produce a large error in the estimate of the n'th polynomial.

As an illustration of the trouble which this introduces in practice, we recall the observation made earlier in this chapter that numerically,

$$\hat{a}^n_\ell \simeq (-1)^\ell \binom{n}{2n-\ell} \hat{a}^n_{2n} . \tag{7.13}$$

With $\hat{a}^n_{2n}$ given by (7.12), it is easy to check algebraically that this is a satisfactory approximate solution to (7.2) when n is large and $\ell \simeq 2n$. There are ways of improving the accuracy of this solution, e.g. by taking the R.H.S. of (7.13) as the first term of a series in which the $(s + 1)$th term is proportional to $\binom{n}{2n-\ell-s}$, the coefficients being found by substitution in (7.2). However such efforts are to no avail in the prediction of accurate values of the polynomials. For if we take the first approximation (7.13) and naïvely extend its validity to the whole range $0 \leqslant \ell \leqslant 2n$ (on the dubious grounds that it predicts at least the numerically largest and seemingly most important coefficients with fair accuracy), we get

$$\sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell \simeq \hat{a}_{2n}^n \sum_{\ell=0}^{2n} (-1)^\ell \binom{n}{2n-\ell} x^\ell$$

$$= \hat{a}_{2n}^n \left[-x(1-x) \right]^n. \tag{7.14}$$

Not only does this completely fail to reproduce the observed oscillations in the n'th polynomial as a function of x, but the magnitude of the two sides of (7.14) are nowhere remotely equal; e.g. when $x = 0.5$ and $n = 7$, the L.H.S. and R.H.S. are equal to 1.134 and 499.9 respectively.

The difficulties described are not appreciably reduced by changing to the independent variable X. In place of (7.2) we have a recurrence relation for the new coefficients $\hat{A}_\ell^n$ derived from (6.19) by retaining only the t = 1 term:

$$\hat{A}_\ell^n = -\frac{\rho}{4}\hat{A}_{\ell-1}^{n-1} + \frac{1}{9}\hat{A}_\ell^{n-1} + \frac{\mu}{2}\left[\binom{2\ell}{2}\hat{A}_{\ell-1}^{n-1} - 2\binom{2\ell+1}{2}\hat{A}_\ell^{n-1} + \binom{2\ell+2}{2}\hat{A}_{\ell+1}^{n-1} \right]. \tag{7.15}$$

Putting $\ell = 0$, we see that $\hat{A}_0^n$ is expressed in terms of $\hat{A}_0^{n-1}$ <u>and</u> $\hat{A}_1^{n-1}$ so, unlike $\hat{a}_0^n$, cannot be derived as an exact special case. Putting $\ell = n$, we get almost the same equation as for $\hat{a}_{2n}^n$ and consequently encounter just the same difficulties.

Ideally we require an approximate solution for $\hat{A}_\ell^n$ for small ℓ, since this would yield accurate values of the polynomials in the representative region $X \simeq 0$. The obstacles to finding an analytic solution do not of course prevent an attempt to find a solution by numerical methods. If resorted to, however, one might just as well examine straightaway the form of A_ℓ^n and pay no further attention to $\hat{A}_\ell^n$. This is done in Chapter 8.

7.2 Second Method: Construction of the Differential Equation for $\hat{\psi}$.

We first prove $\hat{\psi}(x)$ to be the solution of an inhomogeneous differential equation of second order. Combining (7.2) and (7.6),

$$\hat{\psi}(x) = 1 + \sum_{n=1}^{\infty} y^{2n} \sum_{\ell=0}^{2n} x^\ell \left\{ -\tfrac{1}{18}\hat{a}_\ell^{n-1} + \tfrac{2}{3}\hat{a}_{\ell-1}^{n-1} - \tfrac{2}{3}\hat{a}_{\ell-2}^{n-1} + \mu(\ell+1)\left[\ell\,\hat{a}_\ell^{n-1} - 2(\ell-1)\hat{a}_{\ell-1}^{n-1} + (\ell-2)\hat{a}_{\ell-2}^{n-1}\right]\right\}$$

$$= 1 + y^2 \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n+2} x^\ell \left\{ -\tfrac{1}{18}\hat{a}_\ell^{n} + \tfrac{2}{3}\hat{a}_{\ell-1}^{n} - \tfrac{2}{3}\hat{a}_{\ell-2}^{n} + \mu(\ell+1)\left[\ell\,\hat{a}_\ell^{n} - 2(\ell-1)\hat{a}_{\ell-1}^{n} + (\ell-2)\hat{a}_{\ell-2}^{n}\right]\right\}$$

$$= 1 + y^2\left(-\tfrac{1}{18} + \tfrac{2}{3}x - \tfrac{2}{3}x^2\right)\hat{\psi}(x) + \mu y^2 \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n+2} x^\ell(\ell+1)\left[\ell\,\hat{a}_\ell^{n} - 2(\ell-1)\hat{a}_{\ell-1}^{n} + (\ell-2)\hat{a}_{\ell-2}^{n}\right]. \tag{7.16}$$

Now

$$\sum_{\ell=0}^{2n+2} \hat{a}_\ell^n (\ell+1)\ell\, x^\ell = x \frac{d^2}{dx^2}\, x \sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell ,$$

$$\sum_{\ell=0}^{2n+2} \hat{a}_{\ell-1}^n (\ell+1)(\ell-1)\, x^\ell = x^2\left(\frac{d^2}{dx^2}x + \frac{d}{dx}\right)\sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell, \tag{7.17}$$

$$\sum_{\ell=0}^{2n+2} \hat{a}_{\ell-2}^n (\ell+1)(\ell-2)\, x^\ell = x^3\left(\frac{d^2}{dx^2}x + 2\frac{d}{dx}\right)\sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell ,$$

whereupon (7.16) quickly reduces to

$$\hat{\psi}(x)\left[1+y^2\left(\tfrac{1}{18}-\tfrac{2}{3}x+\tfrac{2}{3}x^2\right)\right] = 1+\mu y^2\left[x^2(1-x)^2\frac{d^2\hat{\psi}}{dx^2}+2x(1-x)(1-2x)\frac{d\hat{\psi}}{dx}\right]. \tag{7.18}$$

The solution of this equation will shortly be found in the two forms (i) as an integral representation (§ 7.4) and (ii) as a convergent infinite series (§ 7.5). Before doing this, however, it is interesting to demonstrate (§ 7.3) that (7.18) is the first order approximation to an infinite order differential equation obtained from the original integral equation (3.9).

7.3 The Infinite Order Differential Equation for $\psi(x)$

We first rewrite the original integral equation (3.9) as

$$\psi(x)\int_{-y}^{y}\frac{dz\; z^4}{[x+e^{z}(1-x)]\,|1-e^{-z}|} = \tfrac{1}{2}y^4+\int_{-y}^{y}\frac{dz\; z^2\,(\rho y^2-z^2)}{[x+e^{z}(1-x)]\,|1-e^{-z}|}\left\{\psi\left[\frac{x}{x+e^{z}(1-x)}\right]-\psi(x)\right\} \tag{7.19}$$

or, since $\psi(x) = \psi(1-x)$,

$$\psi(x)\int_{-y}^{y}\frac{dz\; z^4}{|z|\,(xe^{-z}+1-x)}\left(\frac{z}{e^{z}-1}\right) = \tfrac{1}{2}y^4+\int_{-y}^{y}\frac{dz\; z^2\,(\rho y^2-z^2)}{|z|\,(xe^{-z}+1-x)}\left(\frac{z}{e^{z}-1}\right)\left[\psi\left(\frac{1-x}{xe^{-z}+1-x}\right)-\psi(1-x)\right]. \tag{7.20}$$

As a special case of the result established in (3.17),

$$\frac{1}{xe^{-z}+1-x}\left(\frac{z}{e^{z}-1}\right) = \sum_{\ell=0}^{\infty}\frac{(-z)^{\ell}}{\ell!}\sum_{\nu=0}^{\ell}(-1)^{\nu}\nu!\,\frac{\ell}{\nu}\,C_{\ell}^{\nu}\,x^{\nu}. \tag{7.21}$$

The integral on the L.H.S. of (7.20) involves

$$\int_{-y}^{y} \frac{dz\, z^{\ell+4}}{|z|} = 2\, y^{\ell+4}/(\ell+4) \quad , \ \ell \text{ even}, \qquad (7.22)$$
$$= 0 \qquad , \ \ell \text{ odd}.$$

The L.H.S. of (7.20) therefore equals

$$\psi(x)\, \tfrac{1}{2} y^4 \sum_{t=0}^{\infty} \frac{y^{2t}}{(2t)!} \frac{4}{2t+4} \sum_{v=0}^{2t} (-1)^v v!\, \frac{2t}{v}\, C^{v}_{2t}\, x^{v} \,. \qquad (7.23)$$

Turning to the R.H.S. of (7.20), our main problem is to expand the quantity in the square brackets in rising powers of z. Once again we apply the recipe (3.12), yielding

$$\psi\left(\frac{1-x}{xe^{-z}+1-x}\right) - \psi(1-x) = \sum_{n=1}^{\infty} \frac{(-z)^n}{n!} \sum_{v=1}^{n} C^{v}_{n} \left(\frac{d}{dy}\right)^{v} \psi\left(\frac{1-x}{xy+1-x}\right)\Big|_{y=1} \,. \qquad (7.24)$$

It is now helpful to choose a temporary new variable

$$W = \frac{1-x}{xy+1-x} \,, \qquad (7.25)$$

whereupon Schlömilch's formula[39] enables us to write

$$\left(\frac{d}{dy}\right)^{v} \psi(W) = \sum_{r=0}^{v} S_{vr}\, \psi^{(r)}(W) \qquad (7.26)$$

where

$$S_{vr} = \frac{v!}{r!} \times \text{coeff. of } \varepsilon^{v} \text{ in } \left[\frac{1-x}{x(y+\varepsilon)+1-x} - \frac{1-x}{xy+1-x}\right]^{r}$$

$$= \frac{v!}{r!} \frac{[-x(1-x)]^{r}}{[xy+1-x]^{r}} \times \text{coeff. of } \varepsilon^{v-r} \text{ in } \frac{1}{(1-x+xy+x\varepsilon)^{r}}$$

$$= \frac{\nu!}{r!}\frac{(-1)^\nu x^\nu (1-x)^r}{(xy+1-x)^{\nu+r}}\binom{\nu-1}{r-1}.$$

(7.27)

Hence, putting $y = 1$,

$$\psi\left(\frac{1-x}{xe^{-z}+1-x}\right) - \psi(1-x) =$$

$$= \sum_{n=1}^{\infty}\frac{(-z)^n}{n!}\sum_{\nu=1}^{n} C_n^\nu \sum_{r=1}^{\nu}\left[\frac{d}{d(1-x)}\right]^r \psi(1-x)\frac{\nu!}{r!}(-1)^\nu x^\nu (1-x)^r\binom{\nu-1}{r-1}$$

$$= \sum_{n=1}^{\infty}\frac{(-z)^n}{n!}\sum_{r=1}^{n}(-1)^r\psi^{(r)}(x)\frac{(1-x)^r}{r!}\sum_{\nu=r}^{n} C_n^\nu\, \nu!(-1)^\nu\binom{\nu-1}{r-1}x^\nu$$

$$= \sum_{n=1}^{\infty}\frac{(-z)^n}{n!}\sum_{r=1}^{n}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{s=0}^{n-r} C_n^{r+s}(r+s)!(-1)^s\binom{r+s-1}{s}x^s.$$

(7.28)

Combining (7.21) and (7.28), the integral on the R.H.S. of (7.20) is proportional to

$$\sum_{\ell=0}^{\infty}\frac{(-z)^\ell}{\ell!}\sum_{\nu=0}^{\ell}(-1)^\nu \nu!\frac{\ell}{\nu}C_\ell^\nu x^\nu\sum_{n=1}^{\infty}\frac{(-z)^n}{n!}\sum_{r=1}^{n}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{s=0}^{n-r}C_n^{r+s}(r+s)!(-1)^s\binom{r+s-1}{s}x^s$$

$$= \sum_{m=1}^{\infty}\frac{(-z)^m}{m!}\sum_{n=1}^{m}\binom{m}{n}\sum_{\nu=0}^{m-n}(-1)^\nu \nu!\frac{m-n}{\nu}C_{m-n}^\nu x^\nu\sum_{r=1}^{n}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{s=0}^{n-r}C_n^{r+s}(r+s)!(-1)^s\binom{r+s-1}{s}x^s$$

$$= \sum_{m=1}^{\infty}\frac{(-z)^m}{m!}\sum_{r=1}^{m}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{n=r}^{m}\binom{m}{n}\sum_{\nu=0}^{m-n}(-1)^\nu \nu!\frac{m-n}{\nu}C_{m-n}^\nu x^\nu\sum_{s=0}^{n-r}C_n^{r+s}(r+s)!(-1)^s\binom{r+s-1}{s}x^s.$$

(7.29)

Now

$$\sum_{n=r}^{m}\sum_{\nu=0}^{m-n}\sum_{s=0}^{n-r} = \sum_{\nu=0}^{m-r}\sum_{s=0}^{m-\nu-r}\sum_{n=r+s}^{m-\nu} \tag{7.30}$$

and, from (A1.34) of Appendix 1,

$$\sum_{n=r+s}^{m-\nu} \binom{m}{n}(m-n)\, C_{m-n}^{\nu}\, C_{n}^{r+s} = m\binom{\nu+r+s-1}{\nu-1} C_{m}^{\nu+r+s}. \tag{7.31}$$

Hence (7.29) is equal to

$$\sum_{m=1}^{\infty}\frac{(-z)^m}{m!}\sum_{r=1}^{m}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{\nu=0}^{m-r}(-1)^{\nu}(\nu-1)!\,x^{\nu}\sum_{s=0}^{m-\nu-r}(r+s)!(-1)^s\binom{r+s-1}{s}x^s\, m\binom{\nu+r+s-1}{\nu-1}C_m^{\nu+r+s}$$

$$=\sum_{m=1}^{\infty}\frac{(-z)^m}{m!}\sum_{r=1}^{m}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{\ell=0}^{m-r}x^{\ell}(-1)^{\ell}\sum_{s=0}^{\ell}(\ell-s)!(r+s)!\binom{r+s-1}{s}\binom{\ell+r}{\ell-s}\frac{m}{\ell+r}C_m^{\ell+r}$$

$$=\sum_{m=1}^{\infty}\frac{(-z)^m}{m!}\sum_{r=1}^{m}\frac{\psi^{(r)}(x)[x(1-x)]^r}{r!}\sum_{\ell=0}^{m-r}x^{\ell}(-1)^{\ell}(\ell+r)!\binom{r+\ell}{\ell}\frac{m}{\ell+r}C_m^{\ell+r}. \tag{7.32}$$

The integration over z involves

$$\int_{-y}^{y}\frac{dz\; z^{m+2}}{|z|}(\rho y^2-z^2) = 2y^{m+4}\left(\frac{\rho}{m+2}-\frac{1}{m+4}\right), \quad m \text{ even}$$

$$= 0 \qquad , \ m \text{ odd} . \tag{7.33}$$

Hence, dividing throughout by $\frac{1}{2}y^4$, (7.20) finally reduces to

$$\psi(x) \sum_{t=0}^{\infty} \frac{y^{2t}}{(2t)!} \frac{4}{2t+4} \sum_{\nu=0}^{2t} (-1)^{\nu} \nu! \frac{2t}{\nu} C_{2t}^{\nu} x^{\nu} = 1$$

$$+ \sum_{t=1}^{\infty} \frac{y^{2t}}{(2t)!} \left(\frac{4\rho}{2t+2} - \frac{4}{2t+4} \right) \sum_{r=1}^{2t} \frac{\psi^{(r)}(x) [x(1-x)]^{r}}{r!} \sum_{\ell=0}^{2t-r} (-x)^{\ell} (\ell+r)! \binom{r+\ell}{\ell} \frac{2t}{\ell+r} C_{2t}^{\ell+r} ,$$

(7.34)

which is the required differential equation.

The zero order approximation $\psi = 1$ results from retention of only the $t = 0$ term in the t-summation, while (7.18) is yielded if terms up to $t = 1$ are retained. The summation index t in (7.34) therefore plays the same role as the same index in (3.23).

Similar equations result if we recast the theory in terms of the variables X and Ψ . At any stage in this chapter it is straightforward to replace ψ by Ψ , $\hat{\psi}$ by $\hat{\Psi}$ and x by $\frac{1}{2}(1-X)$ to find equivalent relations.

7.4 Solution for $\hat{\psi}$ as an Integral Representation

As a preliminary, we change to the new variable

$$t = 4x(1-x) , \qquad (7.35)$$

so that the relevant range of t is $0 \leqslant t \leqslant 1$. Putting

$$\hat{\psi}(x) = A(t) , \qquad (7.36)$$

the differential equation (7.18) takes the more convenient form

$$2(1-t)t^2 \ddot{A} + (4-5t)t\dot{A} - (\alpha - \gamma t)A + \beta = 0 , \qquad (7.37)$$

where

$$\alpha = \frac{2}{\mu y^2}\left(1 + \tfrac{1}{18} y^2\right), \quad \beta = \frac{2}{\mu y^2}, \quad \gamma = \frac{1}{3\mu}, \tag{7.38}$$

and a dot indicates differentiation with respect to t. The boundary conditions to be imposed are found by first solving (7.2) for $\hat{a}_0^n$ and $\hat{a}_1^n$. Already in (7.11) we have the solution for $\hat{a}_0^n$. For $\hat{a}_1^n$ the recurrence relation is

$$\hat{a}_1^n = \left(-\tfrac{1}{18} + 2\mu\right) \hat{a}_1^{n-1} + \tfrac{2}{3} \hat{a}_0^{n-1}, \tag{7.39}$$

whose solution is

$$\hat{a}_1^n = \frac{1}{3\mu}\left[\left(-\tfrac{1}{18} + 2\mu\right)^n - \left(-\tfrac{1}{18}\right)^n \right]. \tag{7.40}$$

Hence

$$\hat{\psi}(0) = \sum_{n=0}^{\infty} y^{2n} \hat{a}_0^n = \frac{1}{1 + \frac{1}{18} y^2}, \tag{7.41}$$

$$\hat{\psi}'(0) = \sum_{n=1}^{\infty} y^{2n} \hat{a}_1^n = \frac{\frac{2}{3} y^2}{\left(1 + \frac{1}{18} y^2\right)\left[1 + \left(\frac{1}{18} - 2\mu\right) y^2\right]}. \tag{7.42}$$

In terms of the new function A(t),

$$A(0) = \beta/\alpha, \qquad \dot{A}(0) = \frac{\beta\gamma}{\alpha(\alpha - 4)}. \tag{7.43}$$

The first step in finding an integral representation for A(t) is to solve the homogeneous equation derived from (7.37) by omitting the β term. The exponents of the singularity at t = 0 are

$$c_{\pm} = \frac{1}{2}\left[-1 \pm (1+2\alpha)^{1/2}\right], \tag{7.44}$$

whereas the corresponding exponents of the singularity at t = 1 are 0 and $\frac{1}{2}$. Hence, to convert the original homogeneous equation into standard hypergeometric form, we write

$$A(t) = t^{c_+} u(t), \tag{7.45}$$

which yields the following differential equation for u :

$$(1-t)t\ddot{u} + \left[(2c_+ + 2) - (5/2 + 2c_+)t\right]\dot{u} + (\gamma/2 - \tfrac{3}{2}c_+ - c_+^2)u = 0. \tag{7.46}$$

One solution of the homogeneous equation is therefore

$$A_0(t) = t^{c_+} F(a, b; c; t) \tag{7.47}$$

where

$$\left.\begin{matrix} a \\ b \end{matrix}\right\} = \frac{1}{4} + \frac{1}{2}(1+2\alpha)^{1/2} \pm \frac{1}{4}(9+8\gamma)^{1/2}, \tag{7.48}$$

$$c = 1 + (1+2\alpha)^{1/2}, \tag{7.49}$$

and F is the hypergeometric function.

To find the solution of the inhomogeneous equation we next substitute

$$A(t) = A_0(t)\,v(t) \tag{7.50}$$

in (7.37), yielding

$$(1-t)\, t\, F\, \ddot{\upsilon} + \left\{ 2(1-t)\, t\, \dot{F} + \left[c - (a+b+1)\, t \right] F \right\} \dot{\upsilon} = -\frac{\beta}{2}\, t^{c_-} . \tag{7.51}$$

One integration can now be effected by the method of integrating factors, resulting in

$$\dot{\upsilon}\, F^2\, t^c \sqrt{1-t} = -\frac{\beta}{2} \int^{t} \frac{F(a,b;c;x)\, x^{c_+}\, dx}{\sqrt{1-x}} . \tag{7.52}$$

It may be shown that the boundary condition for $\dot{A}$ (0) is incorporated by setting the lower limit of integration equal to zero. Integrating again, and substituting the resulting expression for $\upsilon(t)$ back into (7.50), the required solution is

$$A(t) = -\frac{\beta}{2}\, t^{c_+}\, F(a,b;c;t) \int_0^t \frac{dy}{F^2(a,b;c;y)\, y^c \sqrt{1-y}} \int_0^y \frac{F(a,b;c;x)\, x^{c_+}\, dx}{\sqrt{1-x}} , \tag{7.53}$$

where the boundary condition for A(0) is likewise incorporated by setting to zero the other lower limit of integration.

From (7.48) and (7.49), $c = a + b + \frac{1}{2}$. In consequence,

$$F(a,b;c;x) = 2^{c-1}\, \Gamma(c)\, x^{\frac{1-c}{2}}\, P^{1-c}_{a-b-\frac{1}{2}}\left(\sqrt{1-x}\right) , \tag{7.54}$$

where P^{ℓ}_{m} is the associated Legendre function of the first kind[33]. Hence (7.53) may alternatively be written as

$$A(t) = -\frac{\beta}{2}\, \frac{P^{-\mu}_{\nu}(\sqrt{1-t})}{\sqrt{t}} \int_0^t \frac{dy}{y\sqrt{1-y}\left[P^{-\mu}_{\nu}(\sqrt{1-y})\right]^2} \int_0^y \frac{P^{-\mu}_{\nu}(\sqrt{1-x})\, dx}{\sqrt{x(1-x)}} , \tag{7.55}$$

where

$$\mu = (1+2\alpha)^{1/2} , \qquad \nu = \tfrac{1}{2}(9+8\gamma)^{1/2} - \tfrac{1}{2} . \tag{7.56}$$

Although these expressions for A(t) are exact, they are extremely inconvenient for numerical evaluation. We proceed therefore to find a solution for A in series form, more suited to numerical computation.

7.5 Solution for $\hat{\Psi}$ in Series Form

Starting again from (7.37), we substitute

$$A(t) = \sum_{r=0}^{\infty} a_r t^r , \tag{7.57}$$

and equate to zero coefficients of successive powers of t on the L.H.S. This produces

$$a_0 = \beta/\alpha \tag{7.58}$$

and, for $r \geqslant 1$,

$$a_r = a_{r-1} \frac{2r^2 - r - 1 - \gamma}{2r^2 + 2r - \alpha} , \qquad \alpha \neq 2r(r+1) . \tag{7.59}$$

The series (7.57) is absolutely convergent for $0 \leqslant t \leqslant 1$, the whole of the range of interest. The boundary conditions (7.43) are obviously satisfied by this solution and, it should be noted, would not generally remain so if there were added on to this solution any linear combination of the two solutions of the corresponding homogeneous equation. Although the differential equation (7.37) has singularities at t = 0 and t = 1, the solution we have obtained is analytic everywhere in the range $0 \leqslant t \leqslant 1$.

The convergence of the series (7.57) may be improved by the following procedure. The recurrence relation (7.59) is first solved to give

$$a_r = \frac{\beta}{\alpha}\,\frac{(-c_-)!\,(-c_+)!}{(-d_-)!\,(-d_+)!}\,\frac{(r-d_-)!\,(r-d_+)!}{(r-c_-)!\,(r-c_+)!}\,, \tag{7.60}$$

where $c_\pm$ are given in (7.44) and

$$d_\pm = \tfrac{1}{4} \pm \tfrac{1}{4}\left(9+8\gamma\right)^{1/2}. \tag{7.61}$$

Since

$$(d_+ + d_-) - (c_+ + c_-) = 3/2\,, \tag{7.62}$$

and, when r is large,

$$(r+a)! \simeq r!\,r^a, \tag{7.63}$$

$$\frac{(r-d_-)!\,(r-d_+)!}{(r-c_-)!\,(r-c_+)!} \simeq \frac{(r-3/2)!}{r!}\,. \tag{7.64}$$

The R.H.S. is the first term in an asymptotic expansion of the L.H.S., of the form

$$\frac{(r-d_-)!\,(r-d_+)!}{(r-c_-)!\,(r-c_+)!} = \frac{(r-3/2)!}{r!}\left\{1 + \frac{F_1}{r+1} + \frac{F_2}{(r+1)(r+2)} + \frac{F_3}{(r+1)(r+2)(r+3)} + \cdots\right\}, \tag{7.65}$$

where expressions for coefficients F_i will shortly be derived. Breaking off the series at the (s+1)th term, we define

$$a_r^* = \frac{\beta}{\alpha}\,\frac{(-c_-)!\,(-c_+)!}{(-d_-)!\,(-d_+)!}\,\frac{(r-3/2)!}{r!}\left\{1 + \frac{F_1}{r+1} + \frac{F_2}{(r+1)(r+2)} + \cdots + \frac{F_s}{(r+1)(r+2)\cdots(r+s)}\right\}. \tag{7.66}$$

The difference between a_r and a_r^* is therefore of order $r^{-(s+3/2)}$ when r is large. Now

$$A(t) = \sum_{r=0}^{\infty} a_r^* t^r + \sum_{r=0}^{\infty} (a_r - a_r^*) t^r$$

$$= \frac{\beta}{\alpha} \frac{(-c_-)!(-c_+)!}{(-d_-)!(-d_+)!} (-\tfrac{3}{2})! \Big\{ (1-t)^{1/2} + \frac{F_1}{(-3/2)t} \left[(1-t)^{3/2} - 1 \right] + \frac{F_2}{(-3/2)(-\frac{5}{2})t^2} \left[(1-t)^{5/2} - 1 + \tfrac{5}{2}t \right]$$

$$+ \cdots + \frac{F_s}{(-\frac{3}{2})(-\frac{5}{2})\cdots(-s-\frac{1}{2})t^s} \left[(1-t)^{s+\frac{1}{2}} - \sum_{n=0}^{s-1} \binom{s+\frac{1}{2}}{n} (-t)^n \right] \Big\} + \sum_{r=0}^{\infty} (a_r - a_r^*) t^r ,$$

(7.67)

and the only infinite series now appearing on the R.H.S. is rapidly convergent.

It remains to calculate the coefficients F_n . Taking the natural logarithm of both sides of (7.65) and noting[46] that

$$\ln(r+a-1)! = (r+a-\tfrac{1}{2})\ln r - r + \tfrac{1}{2}\ln 2\pi + \frac{B_2(a)}{1.2}\frac{1}{r} - \frac{B_3(a)}{2.3}\frac{1}{r^2} + \cdots$$

(7.68)

where $B_n(a)$ is the n'th Bernoulli polynomial, and that

$$B_n(1-a) = (-1)^n B_n(a) , \tag{7.69}$$

$$\ln \left[1 + \frac{F_1}{r+1} + \frac{F_2}{(r+1)(r+2)} + \frac{F_3}{(r+1)(r+2)(r+3)} + \cdots \right] =$$

$$= \frac{G_1}{r} + \frac{G_2}{r^2} + \frac{G_3}{r^3} + \cdots\cdots , \tag{7.70}$$

where

$$G_n = \frac{1}{n(n+1)}\left[B_{n+1}(d_-) + B_{n+1}(d_+) - B_{n+1}(c_-) - B_{n+1}(c_+) - B_{n+1}(3/2) + B_{n+1}(0)\right]. \tag{7.71}$$

Putting $x = 1/r$, this is the same as

$$G_1 x + G_2 x^2 + \ldots = \ln\left[1 + \frac{F_1 x}{1+x} + \frac{F_2 x^2}{(1+x)(1+2x)} + \cdots\right] \tag{7.72}$$

$$= \ln\left[1 + H_1 x + H_2 x^2 + \cdots\right],$$

where (see Jordan[30], p. 175)

$$H_n = (-1)^n \sum_{r=1}^{n} (-1)^r C_n^r F_r . \tag{7.73}$$

Expanding the R.H.S. of (7.72) in rising powers of x, equating coefficients and solving for H_n,

$$H_1 = G_1 ,$$

$$H_2 = G_2 + \frac{1}{2} G_1^2 ,$$

$$H_3 = G_3 + G_1 G_2 + \frac{1}{6} G_1^3 ,$$

$$H_4 = G_4 + G_1 G_3 + \frac{1}{2} G_2^2 + \frac{1}{2} G_1^2 G_2 + \frac{1}{24} G_1^4 ,$$

$$\vdots$$

$$H_n = \sum_{p_1, p_2 \ldots p_n} \frac{G_n^{p_n} G_{n-1}^{p_{n-1}} \cdots G_2^{p_2} G_1^{p_1}}{p_n! \, p_{n-1}! \cdots p_2! \, p_1!} , \tag{7.74}$$

where the sum is over all combinations of integers p_s satisfying

$$\sum_{s=1}^{n} s\,p_s = n \; . \tag{7.75}$$

Combining (7.73) and (7.74),

$$F_1 = G_1 \, ,$$

$$F_n = \sum_{\substack{p_1, p_2 \ldots p_n \\ (\sum s p_s = n)}} \frac{G_n^{p_n} G_{n-1}^{p_{n-1}} \ldots G_2^{p_2} G_1^{p_1}}{p_n! \, p_{n-1}! \ldots p_2! \, p_1!} - (-1)^n \sum_{r=1}^{n-1} (-1)^r C_n^r F_r \, , \quad n \geqslant 2 . \tag{7.76}$$

It is interesting to note in passing that the expansion (7.65) may be generalised as follows:

$$\frac{(r-\alpha_1)! \ldots (r-\alpha_\ell)!}{(r-\beta_1)! \ldots (r-\beta_\ell)!} = \frac{(r-\alpha_1 \ldots -\alpha_\ell + \beta_1 \ldots + \beta_\ell)!}{r!} \left[1 + \frac{F_1}{r+1} + \frac{F_2}{(r+1)(r+2)} + \ldots \right] \tag{7.77}$$

where the F's are given by (7.76) and the G's by

$$G_n = \frac{1}{n(n+1)} \left[B_{n+1}(\alpha_1) + \ldots + B_{n+1}(\alpha_\ell) - B_{n+1}(\beta_1) \ldots - B_{n+1}(\beta_\ell) - B_{n+1}(\alpha_1 + \ldots - \beta_\ell) + B_{n+1}(0) \right]. \tag{7.78}$$

Alternatively, the same method may be employed to generalise the result of van Engen's lemma[35] to

$$\frac{(r-\alpha_1)! \ldots (r-\alpha_\ell)!}{(r-\beta_1)! \ldots (r-\beta_\ell)!} = r^{-\alpha_1 \ldots + \beta_\ell} \left[1 + \frac{c_1}{r+1} + \frac{c_2}{(r+1)(r+2)} + \ldots \right] \tag{7.79}$$

where the c's are generated by equations of the same form as (7.76), the corresponding G's being given by

$$G_n = \frac{1}{n(n+1)}\left[B_{n+1}(\alpha_1) \cdots + B_{n+1}(\alpha_\ell) - B_{n+1}(\beta_1) \cdots - B_{n+1}(\beta_\ell)\right]. \tag{7.80}$$

7.6 The Relation Between ψ and $\hat{\psi}$

It will now be shown that the function A(t) discussed above is, at best, an approximation to $\psi(x)$ at high but not at low temperatures. In the former limit, $a_0 = \beta/\alpha$ is approximately unity, α and β being individually very large. This ensures [see (7.59)] that $a_r << a_{r-1}$, at least for small values of r , so that A(t) is equal to 1 in zero'th approximation, the property possessed by the exact function $\psi(x)$. At very low temperatures, on the other hand, $y >> 1$ so that $\alpha \doteq$ constant. This means that a_r / a_{r-1} is essentially independent of y, so the dependence of A(t) on temperature is the same as for a_0, which is $\propto y^{-2}$. This contrasts with the known proportionality of $\psi(x)$ to y^4 at very low temperatures [see (2.8)]; there is thus no possibility of $A(t) = \hat{\psi}(x)$ being an adequate approximation to $\psi(x)$ at this end of the temperature range.

The relation between ψ and $\hat{\psi}$ at moderate or high temperatures is established by first noting the approximation established early in this chapter:

$$\sum_{\ell=0}^{2n} a_\ell^n x^\ell \simeq \frac{a_{2n}^n}{\hat{a}_{2n}^n} \sum_{\ell=0}^{2n} \hat{a}_\ell^n x^\ell . \tag{7.81}$$

When p = 1.25, (7.3) and (7.10) yield 7/24 and 0.814860822 for the values of μ and ξ respectively. With these, (5.5)and (7.12) together imply

$$\frac{a^n_{2n}}{\hat{a}^n_{2n}} = - \frac{0.522499 \ \xi!(-\xi-\frac{1}{2})!}{(2.477103006944 49)^n \sqrt{\pi}\ \nu^n}\left[1 + O\left(\frac{1}{n}\right)\right]$$

$$= c\, q^{2n}\left[1 + O\left(\frac{1}{n}\right)\right],$$

(7.82)

where

$$c = 1.157977, \qquad q = 1.07314812265697 \ . \tag{7.83}$$

Recognising explicitly that $\psi(x, y)$ is a function of y as well as of x, the relation between ψ and $\hat{\psi}$ may now be expressed:

$$\psi(x,y) = c\,\hat{\psi}(x, qy) + \sum_{n=0}^{\infty} y^{2n}\left[\sum_{\ell=0}^{2n} a^n_\ell x^\ell - c q^{2n}\sum_{\ell=0}^{2n} \hat{a}^n_\ell x^\ell\right], \tag{7.84}$$

where hopefully the bulk of the R.H.S. is now concentrated in the $c\hat{\psi}$ term, and where it is sufficient to terminate the series in rising powers of y at the least term.

The success of this procedure depends on the extent to which the coefficients in the square bracket in (7.84) are numerically smaller (for a given value of x) than the original coefficients $\sum a^n_\ell x^\ell$. Table 7.3 lists these coefficients for the representative value x = 0.5, and it will be observed that they are considerably smaller than the values of the original coefficients displayed in Table 5.7. Numerical computation of $c\,\hat{\psi}(x, qy)$ for y up to 1.5 and x = 0.5 yields values generally greater than about 2.

n	$\sum_{\ell=0}^{2n} a_\ell^n (.5)^\ell - c\, q^{2n} \sum_{\ell=0}^{2n} \hat{a}_\ell^n (.5)^\ell$
0	-1.5798×10^{-1}
1	-3.7065×10^{-2}
2	-3.3140×10^{-3}
3	-1.8094×10^{-3}
4	1.2172×10^{-3}
5	-2.6486×10^{-3}
6	9.3521×10^{-3}
7	-4.8385×10^{-2}
8	3.4086×10^{-1}
9	-3.1263×10^{0}
10	3.6151×10^{1}

Table 7.3

The smallest term in the series in powers of y in (7.84)is never greater, therefore, than $\sim 1\%$ of the total value of the R.H.S., the major contribution to which is indeed concentrated in the c $\hat{\Psi}$ term. Similar conclusions apply for other values of x. For $y \gtrsim 1.5$ however, the smallest term in the series in (7.84) soon becomes greater than 1% of the value of the R.H.S. and the procedure fails.

Chapter 8

NUMERICAL ANALYSIS OF THE COEFFICIENTS A_ℓ^n AND OF THE ASSOCIATED POLYNOMIALS

As pointed out in the previous chapter, accurate knowledge of the form of the coefficients A_ℓ^n near $\ell = 0$ should enable us to predict with fair accuracy the values of the associated polynomials $\sum_{\ell=0}^{n} A_\ell^n X^{2\ell}$ in the representative region $X \simeq 0$. We now seek this information by numerical analysis of those coefficients A_ℓ^n for which ℓ is small.

It turns out that knowledge of the behaviour of the polynomials in the 'non-physical' region $X > 1$ is of considerable value in guiding the corresponding analysis in the 'physical' region $0 \leqslant X \leqslant 1$. For this reason we will investigate also the form of the coefficients A_ℓ^n near $\ell = n$, those whose contributions increasingly dominate the polynomials as $X \to \infty$.

Once the approximate form of the polynomials in the regions $X \simeq 0$ and $X \to \infty$ has been established, it will be shown how the exercise of intuition supplemented and checked by numerical computation successfully elucidates the approximate form of the polynomials for all values of X. The remaining part of this chapter is devoted to improving the degree of approximation of the expressions obtained and determining the proportionality factors.

8.1 The Form of A_ℓ^n Near $\ell = 0$.

The values of A_ℓ^n at $\ell = 0$ merit proportionately more attention than those for small but <u>non-zero</u> values of ℓ , since the former determine directly the polynomials $\sum A^n_\ell X^{2\ell}$ at X = 0. For this value of X, it might be guessed (rightly, as later evidence confirms) that the form of the polynomial is especially simple. We begin therefore with an analysis of the coefficients A^n_0 .

Recalling the general remarks made in §6.2 about the variation of A^n_ℓ with n, and the proportionality between A^n_n and (2n)! times a constant raised to the power n, our first hypothesis is that the approximate variation of A^n_0 with n might be

$$A^n_0 \propto (2n)!\,\rho^n , \tag{8.1}$$

where ρ is a constant. If this is so,

$$Q_n \equiv \frac{A^n_0}{A^{n-1}_0}\frac{1}{2n(2n-1)} \tag{8.2}$$

should tend to the value ρ as $n \to \infty$. Table 8.1 lists values of Q_n for $6 \leqslant n \leqslant 20$ and shows the surmise to be correct with ρ approximately -0.0340.

These figures do not exclude the possibility of the factorial factor in (8.1) being, more accurately, $(2n + \alpha)!$ with α a constant, since the limiting value for Q_n would then still be ρ . However there would also follow

$$n\left(Q_n/\rho - 1\right) = \alpha + O\left(\tfrac{1}{n}\right) \quad ; \tag{8.3}$$

but, as will shortly be demonstrated, one finds in practice that $n^2\,(Q_n/\rho - 1)$ tends to a constant as $n \to \infty$, indicating the value $\alpha = 0$.

The limit of the sequence in Table 8.1 is best determined by Salzer's extrapolation method[47], the principle of which was explained

n	Q_n
6	-0.03322 89807 88385 4
7	-0.03342 06111 93108 8
8	-0.03355 41979 14926 6
9	-0.03364 93625 89810 6
10	-0.03371 91370 56176 3
11	-0.03377 16695 72261 8
12	-0.03381 21463 70579 2
13	-0.03384 39645 04405 9
14	-0.03386 94138 96056 6
15	-0.03389 00794 99445 5
16	-0.03390 70847 09560 3
17	-0.03392 12428 59166 8
18	-0.03393 31540 71726 9
19	-0.03394 32687 38117 5
20	-0.03395 19300 75444 7

Table 8.1

in §5.1. The 4-point formula based on n = 20 predicts a limit of -0.03403288 whereas the more accurate 7-point formula yields -0.03403388 when n = 15 and -0.03403349 when n = 20. This justifies the conclusion $\rho = -0.0340335$, correct to the last digit included. Evidence will be adduced later in this chapter for the belief that a much more precise estimate of ρ is -0.0340334826863540.

To find a better approximation to A_0^n , we now assume the more general version of (8.1) to be

$$A_0^n = K\,(2n)!\,\rho^n \left[1 + \frac{c}{2n} + O\left(\frac{1}{n^2}\right)\right]. \qquad (8.4)$$

This implies

$$2n^2 (1 - Q_n/\rho) = c + O(\tfrac{1}{n}) , \qquad (8.5)$$

from which c is determined by extrapolating to $1/n = 0$ the sequence of values of the L.H.S. Having found c, K can be similarly evaluated by extrapolating successive values of

$$\frac{A_0^n}{(2n)!\, \rho^n (1 + c/2n)} .$$

To determine c and K with maximum accuracy, the assumed precise value of ρ has been inserted during these calculations.

The results of this procedure are shown in Table 8.2 which lists the extrapolated values resulting from application of the various Salzer formulae. From these, we may reasonably assume the true limits for c and K to be 1.9691 and -0.6652672 respectively, correct to the

Extrapolation formula	Result	
	c	K
n = 20, 4 point	1.96932	-0.6652 6976
n = 15, 7 point	1.96837	-0.6652 6649
n = 20, 7 point	1.96908	-0.6652 6717

<u>Table 8.2</u>

last decimal digit quoted. Summarising, our estimates of the three constants in (8.4) are

$$\begin{aligned} \rho &= -0.0340334826863540 , \\ c &= 1.9691 , \\ K &= -0.6652672 . \end{aligned} \qquad (8.6)$$

We next consider the form of the coefficients A_ℓ^n for small but non-zero values of ℓ. At this stage little information exists about how A_ℓ^n might vary with ℓ, other than that provided by inspection of the appropriate numerical values. There are a number of possible expressions involving factorials and powers which will qualitatively reproduce (for example) the observed initial increase of A_ℓ^n with ℓ; which of these gives the best numerical fit can only be discovered by trial and error. Fortunately we do not have to find the form of A_ℓ^n to the same degree of accuracy as is inherent in (8.4) for A_0^n, even supposing the same accuracy were attainable. Our main interest lies in discovering analytic expressions for the polynomials, and analysis of the coefficients A_ℓ^n is of value only insofar as it helps to achieve this end. The result of this section of the analysis will merely be stated, therefore, with only an outline of its numerical support.

The trial expression for A_ℓ^n which fits the data most accurately is

$$A_\ell^n = K \frac{(2n+2\ell)!}{(2\ell)!} \rho^n \sigma^\ell , \qquad \ell \text{ small} , \tag{8.7}$$

where σ is a constant, approximately equal to -0.40528. When testing this expression against the actual values of A_ℓ^n it is convenient to examine the variations with n and ℓ separately:

(a) <u>Variation with n</u>. Numerical analysis, similar to that already described for $\ell = 0$, confirms that

$$\frac{A_\ell^n}{A_\ell^{n-1}} \; \frac{1}{(2n+2\ell)(2n+2\ell-1)}$$

tends to the value ρ as $n \to \infty$. Assuming the factorial factor in the numerator of (8.7) should more accurately be $[2n + 2\ell + \alpha(\ell)]!$, the demonstration that $\alpha(\ell) = 0$ for $\ell = 1, 2, \ldots$ proceeds along exactly the same lines as led to $\alpha(0) = 0$.

(b) Variation with ℓ. When $\ell = 0$, (8.7) reduces to (8.4) as it must, leaving aside the higher order terms in the latter. Extrapolation to $1/n = 0$ of successive values of

$$\frac{A^n_\ell}{A^n_{\ell-1}} \frac{2\ell(2\ell-1)}{(2n+2\ell)(2n+2\ell-1)}$$

yields the value σ for $\ell = 1, 2, \ldots$.

8.2 The Form of A^n_ℓ Near $\ell = n$

Again we seek a better approximation to A^n_ℓ at the end point of the range for ℓ, this time $\ell = n$, than for neighbouring values. In (6.23) we already have an excellent approximation to A^n_n ; this can still be improved a little however in respect of the accuracy of the proportionality constant, now that values of A^n_ℓ are available up to $n = 20$. Repetition of the argument in § 5.1 leads to an extension of Table 5.4 by eight more entries (from $n = 13$ to $n = 20$) and, by extrapolation, a more precise estimate of -0.522499625 for the proportionality constant. The expression for A^n_n may therefore be written

$$A^n_n = K_1 (2n)! \, \rho_1^n \left[1 + \frac{c_1}{2n} + O\left(\frac{1}{n^2}\right) \right], \qquad (8.8)$$

where

$$\begin{aligned} \rho_1 &= 0.0839742526264095 , \\ c_1 &= 1.631325858441925 , \\ K_1 &= -0.522499625 . \end{aligned} \qquad (8.9)$$

To find the approximate form of A_ℓ^n for neighbouring values of ℓ, we again resort to trial and error checked by numerical computation. The conclusion reached is that the variation of A_ℓ^n with n and ℓ for $\ell \simeq$ n is best represented by

$$A_{n-s}^n = K_1 \frac{(2n+s)!}{s!} \rho_1^n \sigma_1^s \quad , \quad s \text{ small}, \tag{8.10}$$

where σ_1 is a constant approximately equal to -0.33333. This is justified by the observation that

$$\frac{A_{n-s}^n}{A_{n-1-s}^{n-1}} \frac{1}{(2n+s)(2n+s-1)} \quad \text{and} \quad \frac{A_{n-s}^n}{A_{n-s+1}^n} \frac{s}{2n+s}$$

tend respectively to the constants ρ_1 and σ_1 as $n \rightarrow \infty$ for small values of s.

8.3 Approximate Form of the Polynomials for $X \simeq 0$ and $X \rightarrow \infty$

It is convenient at this juncture to denote by $A_n(X)$ the n'th polynomial derived from the coefficients A_ℓ^n, thus:

$$A_n(X) = \sum_{\ell=0}^{n} A_\ell^n X^{2\ell} . \tag{8.11}$$

For very small values of X, $A_n(X)$ is dominated by the contributions associated with A_0^n, A_1^n, A_2^n ... , which are fairly accurately expressed by (8.7). Hence we have, to a good approximation,

$$A_n(X) \simeq K \rho^n \sum_{\ell=0}^{\infty} \frac{(2n+2\ell)!}{(2\ell)!} (\sigma X^2)^\ell$$
$$(X \simeq 0)$$

$$= K(2n)!\,\rho^n(\cos\theta)^{2n+1}\cos(2n+1)\theta\,, \tag{8.12}$$

where

$$\theta = \tan^{-1}[\sqrt{-\sigma}\,X]\,. \tag{8.13}$$

On the other hand, when X becomes very large, $A_n(X)$ is dominated by A^n_n, A^n_{n-1}, A^n_{n-2} ...., which are fairly accurately expressed by (8.10). We then have

$$\underset{(X\to\infty)}{A_n(X)} = \sum_{s=0}^{n} A^n_{n-s}\,X^{2n-2s}$$

$$\simeq K_1\rho_1^n X^{2n}\sum_{s=0}^{\infty}\frac{(2n+s)!}{s!}\left(\sigma_1/X^2\right)^s$$

$$= \frac{K_1}{1-\sigma_1/X^2}(2n)!\,\rho_1^n\left(\frac{X}{1-\frac{\sigma_1}{X^2}}\right)^{2n}. \tag{8.14}$$

It is easy to check numerically that (8.12) and (8.14) are good approximations to $A_n(X)$ for $X \simeq 0$ and $X \to \infty$ respectively, and that they fail for intermediate values of X. Far more important than this, however, is that (8.12) predicts exactly the right <u>form</u> for $A_n(X)$ in the region $0 \leqslant X \leqslant 1$. In Chapter 5 we described how $A_n(X)$ oscillates with variation of X in this region, the amplitude of the oscillation decreasing as X increases from 0, becoming vanishingly small near X = 1, with the period of the oscillation simultaneously increasing. All these features are inherent in (8.12) provided θ is an increasing function of X with values 0 and $\pi/2$ at X = 0 and 1 respectively. The required value at X = 1 is <u>not</u> satisfied by (8.13), of course, but we are entitled to hope that the actual form of A_n (X) when finally elucidated might be hardly more complicated than (8.12), where $\theta(X)$ meets the specification described above and is approximated by (8.13) when X is small. Similarly it is a reasonable expectation that a slightly modified version of (8.14) might be the correct form for A_n (X) for the region $1 < X < \infty$, the principal modification consisting of replacing $X/(1-\sigma_1/X^2)$ by a more general (and, as yet, unknown) function of X, one which reduces to $X(1-\sigma_1/X^2)$ in the limit of very large X. These hypotheses we now put to the test.

8.4 Approximate Form of the Polynomials for All Values of X

Following the discussion of the previous section we assume A_n (X) to be given approximately by

$$A_n(x) \propto (2n)!\, \rho^n (\cos\theta)^{2n} \cos(2n+1)\theta \ , \quad 0 \leq X \leq 1 \ , \qquad (8.15)$$

$$A_n(x) \propto (2n)!\, \rho_1^n\, [h(x)]^{2n} \ , \quad 1 < X < \infty \ , \qquad (8.16)$$

where θ (X) and h(X) are to be determined.

The simplest way to find θ (X) is to locate numerically the zeros of A_n (X). These occur at approximately

$$(2n+1)\,\theta(X) = \frac{\pi}{2} \ , \quad 3\frac{\pi}{2} \ , \quad 5\frac{\pi}{2} \ , \ \cdots \ . \qquad (8.17)$$

[Approximately, because (8.15) is inexact - higher order terms will shift the zeros slightly from these positions.] For given n, (8.17) determines the values $\theta(X_{n1})$, $\theta(X_{n2})\ldots$ corresponding to the observed zeros X_{n1}, $X_{n2}\ldots$ of $A_n(X)$. When we plot all the values of $\theta(X)$ versus X for all the different values of n, a continuous curve will result only if the original hypothesis is correct.

Fig.1 displays the plot of $(2/\pi)\,\theta(X)$ versus X, incorporating data corresponding to values of n between 4 and 20. The curve is quite smooth, and it is easily confirmed that $\theta(X) \simeq \tan^{-1}(\sqrt{-\sigma}\,X)$ for $X \lesssim 0.4$. As $X \to 1$, the gradient of the curve increases rapidly and it is not easy to find the value of $\theta(1)$ by extrapolation; however, the curve is perfectly consistent with our expectation $\theta(1)=\pi/2$.

To find the function h(X) numerically we calculate values of

$$\sqrt{\frac{A_n(X)}{A_{n-1}(X)\,2n(2n-1)\,\rho_1}}$$

for fixed X and variable n and extrapolate to $1/n = 0$, repeating for other values of X. Consistency between the limits predicted by the various Salzer formulae serves as a guide to the true limit for that value of X. Table 8.3 displays the values of $h(X)/X$ for a selection of values of $1/X$. Due to the difficulty of accurately computing high-order $A_n(X)$ near $X = 1$ (at this point numerical cancellation is practically complete) the estimates of h(X) gradually decrease in precision as $1/X$ runs from 0 to 1. The number in brackets after each entry indicates the likely error in the last significant figure quoted. As expected, $h(X)/X \simeq 1/(1-\sigma_1/X^2)$ for $1/X \lesssim 0.5$.

We now require to find the analytic form of $\theta(X)$ and h(X). Happily we possess one important clue to this problem, in the numerical value of the constant which appears in the approximation to h(X) for small $1/X$. Since $\sigma_1 = -0.33333$,

$$h(X) \simeq \frac{X}{1-\frac{\sigma_1}{X^2}} = \frac{1}{\left(\frac{1}{X}\right) + .33333\left(\frac{1}{X}\right)^3}, \quad \frac{1}{X} \text{ small}, \tag{8.18}$$

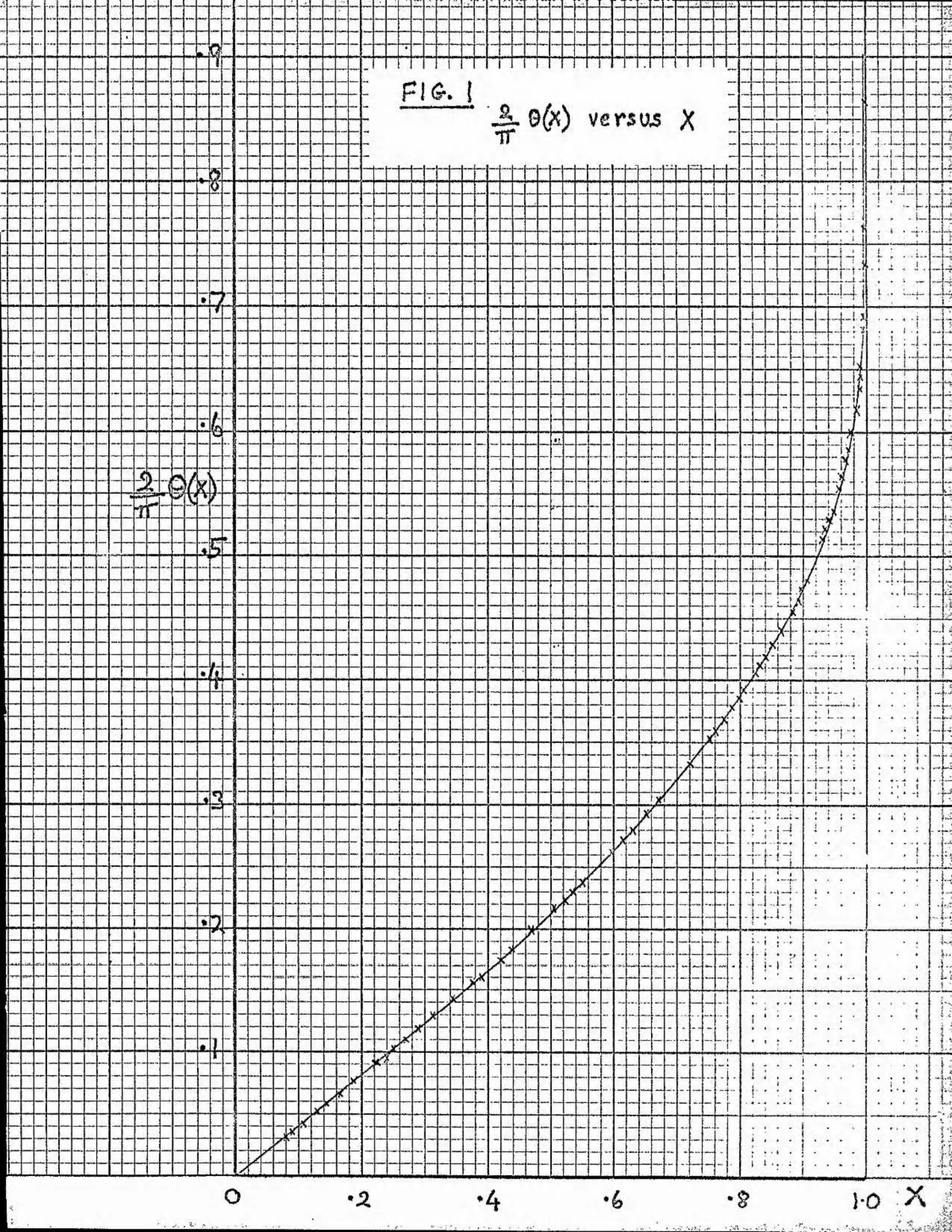


FIG. 1
$\frac{2}{\pi}\theta(X)$ versus X
$\frac{2}{\pi}\theta(X)$
·9
·8
·7
·6
·5
·4
·3
·2
·1
0
·2
·4
·6
·8
1·0
X

$\frac{1}{X}$	$\frac{h(X)}{X}$	$\frac{1}{X \tanh^{-1}(1/X)}$
0.00	1.0	1.0
0.10	0.99665 7731 (1)	0.99665 77309
0.22	0.98365 2988 (3)	0.98365 29883
0.34	0.96020 0998 (5)	0.96020 09988
0.46	0.92497 395 (5)	0.92497 39780
0.54	0.89380 95 (5)	0.89380 94711
0.62	0.85516 6 (1)	0.85516 64125
0.70	0.80710 2 (1)	0.80710 20109
0.78	0.74615 0 (5)	0.74614 69056
0.82	0.70885 (5)	0.70884 13039
0.85	0.6766 (1)	0.67666 92649
0.88	0.6396 (1)	0.63964 28901
0.90	0.6113 (1)	0.61132 18894
0.92	0.5789 (1)	0.57897 06840
0.94	0.5408 (1)	0.54083 61982
0.96	0.4935 (2)	0.49334 24086
0.98	0.4268 (3)	0.42653 94731

Table 8.3

suggesting that $1/h(X)$ can be expressed as a power series in odd powers of X^{-1} commencing $X^{-1} + \frac{1}{3}X^{-3} + \ldots\ldots$. A large number of elementary functions possess this property, but all but one of the most obvious fail to match the numerical values of $h(X)$ given in Table 8.3. The exception is $\tanh^{-1} X^{-1}$, and the hypothesis

$$h(X) = \frac{1}{\tanh^{-1}(1/X)} \tag{8.19}$$

is consistent with both (8.18) and Table 8.3, agreement in the latter case being explicitly demonstrated by inclusion in that table of a list of values of $1/[X \tanh^{-1}(1/X)]$. The conclusion is, therefore, that in the region $1 < X < \infty$,

$$A_n(X) \propto (2n)!\, \rho_1^n \frac{1}{[\tanh^{-1}(1/X)]^{2n}} \tag{8.20}$$

to first approximation.

With this information, it is relatively easy to elicit the analytic form of $\Theta(X)$. Comparing (8.15) with (8.20) in respect of the quantities raised to the power 2n, we see $\sqrt{\rho_1}/\tanh^{-1}(1/X)$ turning into $\sqrt{-\rho}\cos\Theta(X)$ on crossing over from $X > 1$ to $X < 1$. The function $\tanh^{-1}(1/X)$ cannot be expected to carry over as it stands since it has a singularity at $X = 1$. However, since $\tanh^{-1}(1/X) = \pm(\pi/2)i + \tanh^{-1} X$, $\tanh^{-1}(1/X)$ can reasonably be supposed to be replaced by $[\pi^2/4 + (\tanh^{-1} X)^2]^{1/2}$ as we pass from $X > 1$ to $X < 1$, since all the numbers we are dealing with are real. Our surmise then is

$$\sqrt{-\rho}\cos\Theta = \sqrt{\frac{\rho_1}{\pi^2/4 + (\tanh^{-1}X)^2}} \tag{8.21}$$

which, putting $X = 0$, implies $\rho = -4\rho_1/\pi^2$. Taking the exact value of ρ_1 from (8.9), the value of $-4\rho_1/\pi^2$ is -0.0340334826863540 which agrees admirably with our estimate $\rho = -0.0340335$ established independently in §8.1. It is now a simple matter to check that the curve in Fig 1 is an excellent fit to the function

$$\Theta(X) = \cos^{-1}\left[\frac{\pi/2}{\sqrt{\pi^2/4 + (\tanh^{-1}X)^2}}\right]$$

$$= \tan^{-1}\left(\frac{2}{\pi}\tanh^{-1}X\right) . \tag{8.22}$$

The origin of the constant σ in (8.7) and (8.13) is now explained: $\theta(X)$ is approximately $\tan^{-1}(2X/\pi)$ when X is small, and $-\sigma$ therefore equals $4/\pi^2$. The approximate value $-\sigma = 0.40528$ found in § 8.1 agrees excellently with our new analytic prediction of $4/\pi^2 = 0.40528473\ldots$.

To conclude this section, we verify that the two functions each denoted by $\theta(X)$ in (8.15) are one and the same, as has so far been tacitly assumed. To do this we calculate

$$\frac{A_n(X)}{A_{n-1}(X)} \cdot \frac{1}{2n(2n-1)\rho\cos^2\theta} \cdot \frac{\cos(2n-1)\theta}{\cos(2n+1)\theta} \tag{8.23}$$

n	Value of (8.23) for	
	X = 0.10	X = 0.75
8	0.9857	1.0447
9	0.9882	1.0337
10	0.9895	0.9112
11	0.9877	1.0240
12	1.0394	1.0555
13	0.9645	0.9132
14	0.9926	1.0167
15	0.9948	1.1663
16	0.9958	0.8351
17	0.9964	1.0137
18	0.9968	0.8542
19	0.9972	1.1462
20	0.9975	1.0136

Table 8.4

for different values of X and n, the function Θ (X) being given by (8.22). The approximation (8.15) predicts the value unity for (8.23), and this is roughly what is found in practice. Understandably, however, marked deviations from unity occur in the neighbourhood of zeros of $\cos\left[(2n-1)\ \Theta\ (X)\right]$ and $\cos\left[(2n+1)\ \Theta\ (X)\right]$, where the second order terms (to be discussed in the next section) are locally important. These deviations become larger and more frequent as $X \to 1$. This may be attributed partly to the increasing frequency of zeros, and partly to the generally increasing relative magnitude of the second order terms in this region. These features are illustrated in Table 8.4, which lists values of (8.23) for X = 0.10 and 0.75 and n varying between 8 and 20. Allowing for deviations from unity for the reasons given above, the figures amply confirm the validity of the first approximation (8.15).

8.5 The Second Order Terms and Proportionality Factor for $X > 1$

Except for proportionality factors, the expressions (8.15) and (8.20) are the first order approximations to the polynomials $A_n(X)$ in the regions $X < 1$ and $X > 1$ respectively, and suffice when n is very large. We now investigate the form of the second order terms, i.e. those of order $1/n$, and determine the factors of proportionality.

Just as (8.20) is simpler in form than (8.15), so the second order terms for $X > 1$ are more easily investigated than those for $X < 1$. We assume (8.20) to be the first term in an expansion of the form

$$A_n(X) \propto (2n)! \left[\frac{\frac{\pi}{2}\sqrt{-\rho}}{\tanh^{-1}(1/X)}\right]^{2n} \left\{1 + \frac{\beta(X)}{2n} + O\left(\frac{1}{n^2}\right)\right\}, \tag{8.24}$$

where β is a function of X. To find β for any given X, values of

$$2n^2\left[1 - \frac{A_n(X)\left[\tanh^{-1}(1/X)\right]^2 4}{A_{n-1}(X)\,2n(2n-1)(-\rho)\pi^2}\right] = \beta + O(\tfrac{1}{n}) \quad (8.25)$$

corresponding to successive integers n up to 20 are extrapolated to $1/n = 0$ by the Salzer formulae, consistency between the various answers obtained serving as a guide to the true limit for that value of X. Just as for the figures in Table 8.3, the resulting estimates of β (X) steadily decrease in precision as 1/X increases from zero, so much so here that the region $1/X \gtrsim 0.95$ is effectively inaccessible to investigation.

The results are exhibited in Table 8.5 for a selection of values of 1/X in the range 0 to 0.95. As before, the numbers in brackets indicate the probable limits of error in the last decimal digit quoted. Although we cannot calculate $A_n(\infty)$, the value of $\beta(\infty)$ is known from (8.8) and (8.9) to be 1.631325858441925.

From consideration of the form of the first order term in (8.24), we would expect β (X) to be proportional to $\tanh^{-1}(1/X)$ or $[\tanh^{-1}(1/X)]^2$ or perhaps even a combination of both. Direct attempts to fit the data in Table 8.5 by simple functions incorporating one or both of these are somewhat awkward, due mainly to the lack of precision in the known values of β (X) in the region where this function is most rapidly varying. Especially if a number of adjustable parameters are included, it is perfectly possible to find an interpolation formula which, though adequately matching the numerical data in Table 8.5, is nevertheless of quite incorrect <u>analytic</u> form. An example of this type, discovered early on in this investigation by trial and error, is the comparatively simple

$$(b - aX^2)\left[\tanh^{-1}(1/X)\right]^2 + a + 1.631325\ldots \quad ; \qquad (8.26)$$

1/X	β (X)	R.H.S. of (8.27)
0.00	1.631325858441925	1.631325858441925
0.10	1.628762 (1)	1.6287624
0.22	1.618516 (2)	1.6185167
0.34	1.598881 (4)	1.5988826
0.46	1.56627 (3)	1.566275
0.54	1.53383 (5)	1.533850
0.62	1.4881 (2)	1.48814
0.70	1.4208 (5)	1.42092
0.74	1.375 (2)	1.3744
0.78	1.315 (2)	1.3142
0.82	1.234 (3)	1.2334
0.85	1.149 (4)	1.1516
0.88	1.038 (6)	1.0399
0.90	0.935 (8)	0.9388
0.92	0.79 (1)	0.803
0.94	0.59 (3)	0.606
0.95	0.45 (3)	0.468

Table 8.5

with $a = 0.55$ and $b = 0.1124$, this formula provides numerical values in excellent agreement with β (X) except for small discrepancies in the region $1/X \gtrsim 0.85$.

The best method for eliciting the analytic form of β(X) depends on prior knowledge of the proportionality factor in (8.24) yet to be discussed. Although a full description of the details involved must necessarily be postponed, it is convenient to report here the result, that strong evidence points to the correct form of β (X) being

$$\beta(X) = 1.631325\ldots\ X \tanh^{-1}(1/X) - 0.7980398\,[\tanh^{-1}(1/X)]^2 . \tag{8.27}$$

Values of this function are displayed alongside those of $\beta(X)$ in Table 8.5 and agreement is seen to be excellent.

We come now to the question of the proportionality factor in (8.24). This relation, which states the function of n and X to which $A_n(X)$ is proportional for $X > 1$, gives complete information only regarding the variation of $A_n(X)$ with n, as a review of its origin shows. Consequently the factor of proportionality must be assumed a function of X, not just a constant.

From the discussion in § 8.2 on the form of the coefficients A_n^n, the value of the proportionality factor is K_1 (= -0.522499625) for $X \to \infty$. Accordingly we put

$$A_n(X) = K_1\, f(1/X)(2n)! \left[\frac{\frac{\pi}{2}\sqrt{-\rho}}{\tanh^{-1}(1/X)}\right]^{2n} \left\{1 + \frac{\beta(X)}{2n} + O\!\left(\frac{1}{n^2}\right)\right\}, \quad (X > 1) \tag{8.28}$$

so that $f(1/X)$ will reduce to unity at $1/X = 0$. This function is found by direct numerical solution of (8.28), numerical values of all other quantities being inserted up to and including the terms in $1/n$ just discussed*. For given X, this yields a number of estimates of $f(1/X)$ corresponding to different values of n, and the best estimate is obtained by extrapolating these to $1/n = 0$ either via

*To counter the possible charge of circularity, it should be pointed out that in the numerical determination of $f(1/X)$ described here, it hardly matters whether $\beta(X)$ is represented by the analytically correct (8.27), by an interpolation formula such as (8.26) or just by the raw numerical values themselves (i.e. the middle column of figures in Table 8.5). Indeed it is not absolutely necessary to include the second order terms at all - if omitted, the values of $f(1/X)$ can be estimated only with somewhat coarser precision, but the conclusion which is about to be drawn regarding the analytic form of $f(1/X)$ is completely unchanged.

the Salzer formulae or (if inaccuracies in the raw data prevent this) graphically by plotting versus $1/n^2$. Table 8.6 lists the values found for $f(1/X)$ by this process.

$1/X$	$f(1/X)$	$\left[\sqrt{X^2-1}\ \tanh^{-1}(1/X)\right]^{-1}$
0.00	1.0	1.0
0.10	1.0016 78708 (1)	1.0016 78708 0
0.20	1.0068 64173 (1)	1.0068 64172 5
0.30	1.0160 43724 (1)	1.0160 43723 7
0.40	1.0301 8266 (1)	1.0301 82657
0.50	1.0510 538 (2)	1.0510 5373
0.60	1.0820 21 (2)	1.0820 213
0.70	1.1301 71 (5)	1.1301 689
0.80	1.2137 0 (5)	1.2136 52
0.84	1.2678 (1)	1.2677 5
0.88	1.3468 (2)	1.3466 9
0.90	1.4027 (3)	1.4024 7
0.92	1.4775 (5)	1.4772 7
0.94	1.5856 (7)	1.5852 2
0.96	1.762 (1)	1.7619 4
0.97	1.905 (2)	1.9070
0.98	2.140 (5)	2.1434

Table 8.6

We now have to determine the analytic form of $f(1/X)$. Here we are assisted by a criterion whose consequences will be explored more fully in the next section, namely that the expression for $A_n(X)$ valid for $X > 1$ should go over in some simple way to the corresponding expression valid for $X < 1$ as we pass from one region to the other.

Now $\tanh^{-1}(1/X) = \tanh^{-1}X \pm i\frac{\pi}{2}$ which may formally be written as

$$\tanh^{-1}(1/X) = \pm i \frac{\pi}{2} \frac{e^{\mp i\theta}}{\cos\theta} , \qquad (8.29)$$

where θ is defined in (8.22). Since the first order approximation to $A_n(X)$ for $X < 1$ involves $\cos(2n+1)\theta$, it is a fair supposition that $\tanh^{-1}(1/X)$ appearing in (8.28) is actually raised to the power $(2n+1)$ not $2n$, and that the $\cos(2n+1)\theta$ factor then results from taking the real part of $\exp[\pm(2n+1)i\theta]$. We assume therefore that $f(1/X) \propto [\tanh^{-1}(1/X)]^{-1}$. Since the separate factor i in (8.29) will also be raised to the (odd) power $(2n+1)$, it will be helpful if the other factors in $f(1/X)$ yield a purely imaginary quantity as we go from $X > 1$ to $X < 1$. This criterion, together with the conditions (a) $f(0) = 1$, (b) $f(1/X) \to \infty$ as $1/X \to 1$ (strongly suggested by examination of the graphical representation of the data in Table 8.6), (c) $f(1/X) \simeq 1 + \frac{1}{6}(1/X)^2$ for small $1/X$ (the coefficient $\frac{1}{6}$ is suggested by further inspection of the figures in Table 8.6) lead without very great strain of the imagination to the hypothesis

$$f\left(\frac{1}{X}\right) = \frac{1}{\sqrt{X^2-1}\,\tanh^{-1}(1/X)} . \qquad (8.30)$$

This function has all the required properties and, as is demonstrated in Table 8.6, it matches splendidly the numerical values of $f(1/X)$, in every case to within the stated limits of error.

To conclude this section we return to the question of the function $\beta(X)$ and set out the reasons for supposing (8.27) to be correct. Equipped with knowledge of the proportionality factor, it is a straightforward exercise to expand $A_n(X)$ in descending powers of X^2 starting from the term in X^{2n}. In this expansion there is involved

$$\frac{1}{\sqrt{X^2-1}\,\left[\tanh^{-1}(1/X)\right]^{2n+1}} = X^{2n}\left[1 + \frac{g_1}{X^2} + \frac{g_2}{X^4} + \cdots\right] \tag{8.31}$$

where

$$g_1 = \tfrac{1}{2} - \tfrac{1}{3}(2n+1),$$

$$g_2 = \tfrac{3}{8} - \tfrac{11}{30}(2n+1) + \tfrac{1}{18}(2n+1)(2n+2),$$

$$g_3 = \tfrac{5}{16} - \tfrac{103}{280}(2n+1) + \tfrac{17}{180}(2n+1)(2n+2) - \tfrac{1}{162}(2n+1)(2n+2)(2n+3),$$

$$g_4 = \tfrac{35}{128} - \tfrac{1823}{5040}(2n+1) + \tfrac{341}{2800}(2n+1)(2n+2) - \tfrac{23}{1620}(2n+1)(2n+2)(2n+3)$$

$$+ \frac{1}{1944}(2n+1)(2n+2)(2n+3)(2n+4),$$

$$g_5 = \cdots\cdots . \tag{8.32}$$

The corresponding expansion for $\beta(X)$ must be of the form

$$\beta(X) = \beta_0 + \frac{\beta_1}{X^2} + \frac{\beta_2}{X^4} + \cdots\cdots \tag{8.33}$$

where $\beta_0 = 1.631325858441925$, with presumably similar expansions for the higher order terms. The complete expansion for $A_n(X)$ is now

$$A_n(X) = K_1 (2n)! \left(\frac{\pi}{2}\sqrt{-\rho}\right)^{2n} X^{2n} \left[1 + \frac{g_1}{X^2} + \frac{g_2}{X^4} + \cdots\right] \times$$

$$\left[1 + \frac{\beta_0 + \beta_1/X^2 + \beta_2/X^4 + \cdots}{2n} + O\left(\tfrac{1}{n^2}\right)\right]. \tag{8.34}$$

The coefficient of X^{2n} in this expression is of course none other than our original formula (8.8) for A^n_n. However the coefficient of X^{2n-2}, which we know must equal A^n_{n-1}, is

$$A^n_{n-1} = K_1 (2n)! \left(\frac{\pi}{2}\sqrt{-\rho}\right)^{2n} \left\{ g_1\left[1 + \frac{\beta_0}{2n} + O\left(\tfrac{1}{n^2}\right)\right] + \left[\frac{\beta_1}{2n} + O\left(\tfrac{1}{n^2}\right)\right]\right\}$$

$$= g_1 A^n_n + A^n_n \left[\frac{\beta_1}{2n} + O\left(\tfrac{1}{n^2}\right)\right], \tag{8.35}$$

from which

$$\beta_1 = 2n\left[\frac{A^n_{n-1}}{A^n_n} - g_1\right] + O\left(\tfrac{1}{n}\right). \tag{8.36}$$

Similarly from the coefficients of X^{2n-4}, X^{2n-6}, X^{2n-8} ...., which we know must equal A^n_{n-2}, A^n_{n-3}, A^n_{n-4} ..... respectively, we derive

$$\beta_2 = 2n\left[\frac{A^n_{n-2}}{A^n_n} - g_1\frac{A^n_{n-1}}{A^n_n} - (g_2 - g_1^2)\right] + O\left(\tfrac{1}{n}\right),$$

$$\beta_3 = 2n\left[\frac{A^n_{n-3}}{A^n_n} - g_1\frac{A^n_{n-2}}{A^n_n} - (g_2 - g_1^2)\frac{A^n_{n-1}}{A^n_n} - (g_3 - 2g_1 g_2 + g_1^3)\right] + O\left(\tfrac{1}{n}\right),$$

$$\beta_4 = 2n\left[\frac{A^n_{n-4}}{A^n_n} - g_1 \frac{A^n_{n-3}}{A^n_n} - (g_2 - g_1^2)\frac{A^n_{n-2}}{A^n_n} - (g_3 - 2g_1 g_2 + g_1^3)\frac{A^n_{n-1}}{A^n_n} \right.$$

$$\left. - (g_4 - 2g_1 g_3 - g_2^2 + 3g_1^2 g_2 - g_1^4) \right] + O(\tfrac{1}{n}) , \tag{8.37}$$

and so on. Extrapolation to $1/n = 0$ of the R.H.S. of each of these expressions yields

$$\beta_1 = -0.2542645\ (1), \qquad \beta_2 = -0.205762\ (1),$$
$$\beta_3 = -0.174835\ (7), \qquad \beta_4 = -0.15314\ (4). \tag{8.38}$$

It is now possible to select trial analytic expressions for $\beta(X)$ involving $\tanh^{-1}(1/X)$ raised to some low power(s) and, for each, see if the parameters can be adjusted so that the coefficients in the expansion of the function in powers of $(1/X)^2$ exactly correspond to those in (8.38). Naturally it is necessary to employ fewer adjustable parameters than the number of coefficients known (in this case four, excluding β_0) so that a test of the function can properly be made; the hope is that only one or two parameters will prove to be involved.

Since $\beta(X)$ is even in X and tends to the constant β_0 as $1/X \to 0$, it is reasonable to suppose it to be somehow constructed from the following individual terms:

$$\text{constant} \; ; \quad aX\tanh^{-1}(\tfrac{1}{X}) \; ; \quad (b + cX^2)[\tanh^{-1}(\tfrac{1}{X})]^2 \; ; \quad (dX + eX^3)[\tanh^{-1}(\tfrac{1}{X})]^3 . \tag{8.39}$$

(Hopefully, there should be no more complicated expressions playing a role, otherwise the number of parameters would be unwieldy). Combining these in pairs, expanding in rising powers of $(1/X)^2$ and matching coefficients to those in (8.38), complete success is obtained when the second and third are combined with $a = \beta_0$ and $c = 0$. For then we have

$$\beta_0 X \tanh^{-1}\left(\frac{1}{X}\right) + b\left[\tanh^{-1}\left(\frac{1}{X}\right)\right]^2 = \beta_0 + \frac{\frac{1}{3}\beta_0 + b}{X^2} + \frac{\frac{1}{5}\beta_0 + \frac{2}{3}b}{X^4} +$$

$$+ \frac{\frac{1}{7}\beta_0 + \frac{23}{45}b}{X^6} + \frac{\frac{1}{9}\beta_0 + \frac{44}{105}b}{X^8} + O\left(\frac{1}{X^{10}}\right). \tag{8.40}$$

Equating the coefficient of X^{-2} to β_1, $b = -0.7980398$ (1). With this (the only) parameter fixed the next three coefficients are

$$\begin{aligned} \tfrac{1}{5}\beta_0 + \tfrac{2}{3}b &= -0.2057614 \\ \tfrac{1}{7}\beta_0 + \tfrac{23}{45}b &= -0.1748405 \\ \tfrac{1}{9}\beta_0 + \tfrac{44}{105}b &= -0.1531582 \end{aligned} \tag{8.41}$$

which satisfactorily agree with (8.38), allowing for the errors noted.

8.6 The Second Order Terms and Proportionality Factor for $X < 1$

Rather than carry out a similar (but in practice much more awkward) analysis for the second order terms and proportionality factor in the region $X < 1$, it is more profitable to use the corresponding results for $X > 1$ derived in the previous section to predict a trial solution which can then be checked numerically. To do so we apply the criterion that the expression for $A_n(X)$ valid for $X > 1$ should transform into the corresponding form for $X < 1$ when we analytically continue the function $\tanh^{-1}(1/X)$ through the singularity at $X = 1$.

We start from our expression for $A_n(X)$ valid for $X > 1$:

$$A_n(X) = \frac{K_1}{\sqrt{X^2-1}} \frac{(2n)! \left(\frac{\pi}{2}\sqrt{-\rho}\right)^{2n}}{\left[\tanh^{-1}(1/X)\right]^{2n+1}} \left\{ 1 + \frac{\beta_0 X \tanh^{-1}(1/X) + b\left[\tanh^{-1}(1/X)\right]^2}{2n} + O\left(\tfrac{1}{n^2}\right) \right\} . \quad (X>1) \tag{8.42}$$

Taking the upper of the two sign possibilities in (8.29) and noting that $\sqrt{X^2-1} = -i\sqrt{1-X^2}$, this is formally equivalent to

$$A_n(X) = \frac{2K_1}{\pi\sqrt{1-X^2}} (2n)! (\cos\theta)^{2n+1} \rho^n e^{(2n+1)i\theta} \left\{ 1 + \frac{\beta_0 (\pi/2)\, i\, X \sec\theta\, e^{-i\theta} - b(\pi^2/4)\sec^2\theta\, e^{-2i\theta}}{2n} + O\left(\tfrac{1}{n^2}\right) \right\} . \quad (X>1) \tag{8.43}$$

If now X is supposed to be less than 1, the R.H.S. of (8.43) becomes complex, and the expression corresponding to the choice of the lower sign possibility in (8.29) becomes its complex conjugate. Since there is no reason to prefer one sign to the other and since $A_n(X)$ for $X < 1$ is actually real, it is reasonable to suppose it to be derived by adding the two contributions in question, equivalent to taking twice the real part of (8.43). This yields

$$A_n(X) = \frac{4K_1}{\pi\sqrt{1-X^2}} (2n)!\, \rho^n (\cos\theta)^{2n+1} \left\{ \cos(2n+1)\theta + \frac{-\beta_0(\pi/2) X \sec\theta \sin 2n\theta - b(\pi^2/4)\sec^2\theta \cos(2n-1)\theta}{2n} + O\left(\tfrac{1}{n^2}\right) \right\} . \quad (X<1) \tag{8.44}$$

The most readily verifiable constituent of this expression is the outer multiplying constant $4K_1/\pi$. If (8.44) is to reduce to the simple form (8.4) at X = 0, it is necessary that $K = 4K_1/\pi$. Taking the value of K_1 from (8.9), the value of the R.H.S. is found to be -0.665267185 which agrees very well with the estimate K = -0.6652672 established independently in (8.6). From now on the more precise value will be assumed.

Continuing the comparison between (8.4) and the special case of (8.44) for which X = 0, the condition for equality of the second order terms is $c = -b\pi^2/4$. Taking b = -0.7980398 (1) established in the previous section, the R.H.S. is 1.9690843 (2) which is perfectly consistent with the value 1.9691 for c estimated independently in § 8.1*. From now on, the more accurate value will be assumed.

We now examine numerically the second order terms for <u>general</u> values of X and compare them with the prediction (8.44). Here the best procedure is <u>not</u> analogous to that for determining the corresponding quantity for X > 1 (c.f. (8.25)), since the ratio of $A_n(X)$ to $A_{n-1}(X)$ would now involve the quotient of cosines. (In other words the first order term $\cos(2n+1)\theta$ cannot be guaranteed to be dominant over the entire range of X.)

Probably the most efficacious method for isolating the second order terms is simultaneously the most direct. We first write (8.44) in the form

* In retrospect it is evident that the third individual estimate of c in Table 8.2 was more accurate than seemed likely at the time.

$$2n\left\{\frac{A_n(X)\sqrt{1-X^2}}{K(2n)!\,\rho^n(\cos\theta)^{2n+1}} - \cos(2n+1)\theta\right\} =$$

$$= \quad - p(X)\sin 2n\theta + q(X)\cos(2n-1)\theta + O\left(\tfrac{1}{n}\right) \tag{8.45}$$

where, if our hypothesis is correct,

$$p(X) = \beta_0 \frac{\pi}{2} X \sec\theta \quad , \qquad q(X) = -b\frac{\pi^2}{4}\sec^2\theta \; . \tag{8.46}$$

For fixed X, $p(X)$ and $q(X)$ have been determined by extrapolating to $1/n = 0$ the successive estimates of these functions obtained by solving, for successive neighbouring pairs of n-values, the two simultaneous equations which equate the actual numerical values of the L.H.S. of (8.45) to the theoretical form on the R.H.S.

The best estimates of $p(X)$ and $q(X)$ found by this procedure, divided respectively by $X \sec\theta$ and $\sec^2\theta$, are shown in Table 8.7.

X	$\frac{p(X)}{X\sec\theta}$	$\frac{q(X)}{\sec^2\theta}$
0.10	2.6 (1)	1.97 (2)
0.20	2.6 (1)	1.96 (2)
0.40	2.54 (4)	1.98 (2)
0.60	2.55 (3)	1.97 (1)
0.80	2.56 (3)	1.97 (2)
0.90	2.57 (4)	1.97 (2)
0.95	2.57 (4)	1.97 (4)

Table 8.7

Agreement with the theoretical values $\beta_0\pi/2 = 2.56248....$ and $-b\pi^2/4 = 1.96908....$ is once again entirely satisfactory.

It may be noted that we have now automatically verified the outer proportionality factor $\cos\theta/(1-X^2)^{1/2}$ in (8.44). For the success of the above procedure for isolating the second order terms depended critically on this factor being correctly stated; any error here would have caused a large deviation from the proper value of the L.H.S. of (8.45). It is of course possible to check the proportionality factor directly, by the same method which elucidated the numerical variation of $\beta(1/X)$ in the previous section. Although the accuracy in this application is poor compared with the precision of the $\beta(1/X)$ values quoted in Table 8.6, the figures, imprecise though they are, are uniformly consistent with the theoretical form assumed. This evidence will not be adduced however, since the success of the method for eliciting the second order terms provides a much more sensitive test of the proportionality factor in (8.44).

Finally it is necessary to justify the particular choice of $\tanh^{-1}X \pm i\pi/2$ to replace $\tanh^{-1}(1/X)$ in (8.42), and the neglect of the alternative forms $\tanh^{-1}X \pm i3\pi/2$, $\tanh^{-1}X \pm i5\pi/2$, etc., all equally valid through the multivalued nature of the function $\tanh^{-1}$. This is accomplished by showing that each of the additional possible contributions to $A_n(X)$ for $X < 1$ is negligibly small for large values of n and for all but an insignificant range of X. For example,

$$\tanh^{-1}X + i\,3\pi/2 = i\,\frac{\pi}{2}\,\frac{e^{-i\theta}}{\cos\theta}\left[1 + 2\cos\theta\, e^{i\theta}\right], \tag{8.47}$$

the same relation as for $\tanh^{-1}X + i\pi/2$ except for replacing $\cos\theta$ by $\cos\theta/(1+2\cos\theta\, e^{i\theta})$. Since this function is raised to the power 2n+1, the contribution to $A_n(X)$ is, for the representative point X=0, of magnitude $3^{-(2n+1)}$ smaller than those which have been counted hitherto.

Chapter 9

EVALUATION OF Ψ (X)

The late polynomials A_n (X) for X < 1 have now been established to be of the form

$$A_n(x) = \frac{K}{\sqrt{1-x^2}}(2n)!\,\rho^n(\cos\theta)^{2n+1}\left\{\cos(2n+1)\theta\right.$$

$$\left. + \frac{-p(x)\sin 2n\theta + q(x)\cos(2n-1)\theta}{2n} + O\left(\frac{1}{n^2}\right)\right\}$$

$$= \frac{K}{\sqrt{1-x^2}}(2n)!\,\rho^n(\cos\theta)^{2n+1}\,\Re\, e^{i(2n+1)\theta}\left\{1 + \frac{i\,p(x)e^{-i\theta} + q(x)e^{-2i\theta}}{2n} + O\left(\frac{1}{n^2}\right)\right\},$$

(9.1)

where $\Re$ denotes the real part. We are now equipped to carry out the summation over n and thereby find an approximation to

$$\Psi(x) = \sum_{n=0}^{\infty} y^{2n} A_n(x) \; . \tag{9.2}$$

The best way to do this depends on the value attached to y , and we therefore distinguish two procedures appropriate respectively to (a) high and moderate temperatures, and (b) low temperatures.

9.1 Evaluation of Ψ at Moderate and High Temperatures

Since at high temperatures y is reasonably small, successive terms of the summation in (9.2) for $\Psi(X)$ will initially decrease before they eventually increase due to the dominance of the $(2n)!$ factor in $A_n(X)$. We therefore retain s terms exactly and approximate the rest through (9.1), leading to

$$\Psi(X) = \sum_{n=0}^{s-1} y^{2n} A_n(X) + \frac{K\cos\theta}{\sqrt{1-X^2}} \mathcal{R}\, e^{i\theta} \sum_{n=s}^{\infty} \frac{(2n)!}{(-z^2)^n} \times$$

$$\left\{ 1 + \frac{i\,p(X)\,e^{-i\theta} + q(X)\,e^{-2i\theta}}{2n} + O\left(\tfrac{1}{n^2}\right) \right\}, \tag{9.3}$$

where

$$z^{-1} = \sqrt{-p}\; y\cos\theta\; e^{i\theta}. \tag{9.4}$$

Dingle[48] has shown that the late terms in an asymptotic series may be summed provided the n'th term is known and is one of a few standard forms. For the case above, this permits the interpretation

$$\sum_{n=s}^{\infty} \frac{(2n)!}{(-z^2)^n} \longrightarrow \frac{(2s)!}{(-z^2)^s}\, \Pi_{2s}(z) \quad , \quad |\mathrm{ph}\, z| < \pi/2 , \tag{9.5}$$

where the 'converging factor' $\Pi_s(z)$ is defined to be

$$\Pi_s(z) = \frac{1}{s!} \int_0^{\infty} \frac{\varepsilon^s e^{-\varepsilon}\, d\varepsilon}{1 + (\varepsilon/z)^2} . \tag{9.6}$$

Similar interpretations hold for $\sum_{n=s}^{\infty}(2n-1)!/(-z^2)^n$ from the correction term $O(1/n)$ in (9.3), and for corrections of higher order. The final result for Ψ is therefore

$$\Psi(X) = \sum_{n=0}^{s-1} y^{2n} A_n(X) + \frac{K\cos\theta}{\sqrt{1-X^2}} \mathcal{R}\, e^{i\theta} \frac{(2s)!}{(-z^2)^s} \Big\{ \Pi_{2s}(z)$$

$$+ \frac{i\,p(X)\,e^{-i\theta} + q(X)\,e^{-2i\theta}}{2s} \Pi_{2s-1}(z) + O(1/s^2) \Big\}$$

$$= \sum_{n=0}^{s-1} y^{2n} A_n(X) + \frac{K}{\sqrt{1-X^2}} \rho^s (2s)!(\cos\theta)^{2s+1} y^{2s}\, \mathcal{R}\, e^{(2s+1)i\theta} \Big\{ \Pi_{2s}(z)$$

$$+ \frac{i\,p(X)\,e^{-i\theta} + q(X)\,e^{-2i\theta}}{2s} \Pi_{2s-1}(z) + O(1/s^2) \Big\},$$

(9.7)

where it will normally be convenient to break off the series of exact terms at the contribution which is numerically smallest.

Although values of $\Pi_s(z)$ for real z are listed in ref.48, tables for complex z do not yet exist, which raises an obstacle to the numerical evaluation of this expression for general X. However z is real when X = 0 (i.e. $\theta = 0$) and it is then possible to examine the range of y for which a partially - terminated expansion of the above type yields an accurate value of Ψ. This particular choice has the advantage that the polynomials $A_n(X)$ then reduce to the single coefficients A_0^n of particularly simple form, allowing the straightforward numerical determination of some of the higher order terms.

Extending our previous expression (8.4) for A_0^n, we assume

$$A_0^n = K(2n)!\,\rho^n \left[1 + \frac{c}{2n} + \frac{d}{2n(2n-1)} + \frac{e}{2n(2n-1)(2n-2)} + \right.$$

$$\left. + \frac{f}{2n(2n-1)(2n-2)(2n-3)} + \cdots \right] . \tag{9.8}$$

Of the constants c, d, e and f, c is already known from the analysis of the previous chapter to be 1.9690843(2). The others are best determined by extrapolating to $1/n = 0$ the estimates $d(n)$, $e(n)$, $f(n)$ of these quantities defined by

$$c(n) = 2n \left[\frac{A_0^n}{K(2n)!\,\rho^n} - 1 \right],$$

$$d(n) = (2n-1)\left[c(n) - c \right],$$

$$e(n) = (2n-2)\left[d(n) - d \right], \tag{9.9}$$

$$f(n) = (2n-3)\left[e(n) - e \right].$$

The values obtained are

$$c = 1.9690843\ (2)\ , \qquad d = -0.94036\ (8)\ ,$$

$$e = -2.107\ (4)\ , \qquad f = -0.64\ (3)\ . \tag{9.10}$$

Here the estimates of the errors in the later coefficients are based on the supposition that all previous coefficients have been exactly determined; the absolute errors may well be much greater, especially for f.

For $X = 0$, we can now both simplify and extend (9.7) to read

$$\Psi(0) = \sum_{n=0}^{s-1} y^{2n} A_0^n + K\rho^s (2s)!\, y^{2s} \left\{ \Pi_{2s}(z_0) + \frac{c}{2s}\Pi_{2s-1}(z_0) \right.$$

$$\left. + \frac{d\,\Pi_{2s-2}(z_0)}{2s(2s-1)} + \frac{e\,\Pi_{2s-3}(z_0)}{2s(2s-1)(2s-2)} + \frac{f\,\Pi_{2s-4}(z_0)}{2s(2s-1)(2s-2)(2s-3)} + \cdots \right\},$$

(9.11)

where $z_0^{-1} = \sqrt{-\rho}\, y$. For given y, the smallest term in the original asymptotic series determines s, the number of terms to be retained exactly. The correction terms displayed in (9.11) themselves form an asymptotic series which here must necessarily be truncated at the fifth term; the magnitude of this contribution indicates the approximate error in the total value of Ψ.

Table 9.1 lists, for y = 0.5, 1, 2 and 3, the appropriate values of s, $\sum_{n=0}^{s-1} A_0^n y^{2n}$ and the best estimate of $\Psi(0)$. For $y \lesssim 1.0$, $\Psi(0)$

y	s	$\sum_{n=0}^{s-1} A_0^n y^{2n}$	$\Psi(0)$
0.5	6	1.02675179	1.02669062 (6)
1.0	3	1.08942901	1.0998 (2)
2.0	3	1.09753086	1.37 (1)
3.0	2	2.0	1.70 (7)

Table 9.1

is determined with very good accuracy, the error amounting to $\simeq$ 0.02% for y = 1 and rapidly diminishing as y decreases. By y = 2 however the error has increased to $\sim$ 1% and gradually rises as y increases further, amounting to 4% for y = 3.

9.2 Evaluation of $\Psi(X)$ at Low Temperatures

At low temperatures ($y \gg 1$), a clearer description of the variation with temperature of the contributions to Ψ can be given by summing from n = 1 to ∞ over the function found to represent late terms followed by examination of the residual series. We therefore write

$$\underset{(X<1)}{\Psi(X)} = 1 + \frac{K\cos\theta}{\sqrt{1-X^2}} \mathcal{R}\, e^{i\theta} \sum_{n=1}^{\infty} \frac{(2n)!}{(-z^2)^n} \left[1 + \frac{i\,p(X) e^{-i\theta} + q(X) e^{-2i\theta}}{2n} \right]$$

$$+ \sum_{n=1}^{\infty} y^{2n} \left\{ A_n(X) - \frac{K}{\sqrt{1-X^2}} (2n)!\, \rho^n (\cos\theta)^{2n+1} \left[\cos(2n+1)\theta + \frac{-p(X)\sin 2n\theta + q(X)\cos(2n-1)\theta}{2n} \right] \right\}$$

$$(9.12)$$

A standard result[33] is

$$\sum_{n=0}^{\infty} \frac{(2n)!}{(-z^2)^n} = z f(z) \quad , \quad \sum_{n=1}^{\infty} \frac{(2n-1)!}{(-z^2)^n} = -g(z) \quad , \quad |ph\, z| < \pi/2 \, , \tag{9.13}$$

where

$$f(z) = Ci(z)\sin z - si(z)\cos z = \frac{1}{2i}\left[e^{-iz} E_1(-iz) - e^{iz} E_1(iz) \right] , \tag{9.14}$$

$$g(z) = -Ci(z)\cos z - si(z)\sin z = \frac{1}{2}\left[e^{-iz} E_1(-iz) + e^{iz} E_1(iz) \right] . \tag{9.15}$$

Here $Si(z) = si(z) + \pi/2$ and $Ci(z)$ are the sine and cosine integrals and $E_1(z)$ the exponential integral, the definitions of which are

$$Si(z) = \int_0^z \frac{\sin t}{t}\, dt \, , \tag{9.16}$$

$$Ci(z) = \gamma + \ln z + \int_0^z \frac{\cos t - 1}{t}\, dt \quad , \quad |ph\, z| < \pi , \tag{9.17}$$

$$E_1(z) = \int_z^\infty \frac{e^{-t}}{t}\, dt \quad , \quad |ph\, z| < \pi , \tag{9.18}$$

where γ is Euler's constant. The second term on the R.H.S. of (9.12) therefore equals

$$\frac{K\cos\theta}{\sqrt{1-x^2}}\, \mathcal{R}e^{i\theta}\left\{ z\, f(z) - 1 - g(z)\left[\, i\, p(x) e^{-i\theta} + q(x) e^{-2i\theta} \right] \right\} . \tag{9.19}$$

It is now possible to examine the way in which this contribution varies at low temperatures, where $|z| << 1$. The expansions of $Ci(z)$ and $si(z)$ in rising powers of z are

$$Ci(z) = \gamma + \ln z + \sum_{n=1}^{\infty} \frac{(-z^2)^n}{2n(2n)!} \quad , \tag{9.20}$$

$$si(z) = -\frac{\pi}{2} + z \sum_{n=0}^{\infty} \frac{(-z^2)^n}{(2n+1)(2n+1)!} \quad . \tag{9.21}$$

It follows that the dominant terms in $f(z)$ and $g(z)$ for small $|z|$ are

$$f(z) \simeq \frac{\pi}{2} + z(\gamma - 1 + \ln z) \; , \; g(z) \simeq -\gamma - \ln z + \frac{\pi}{2} z , \tag{9.22}$$

which implies that (9.19) is then approximately

$$\frac{K\cos\theta}{\sqrt{1-x^2}}\, \mathcal{R}e^{i\theta}\left\{ \frac{\pi}{2} z - 1 + (\gamma + \ln z - \frac{\pi}{2} z)\left[\, i\, p(x) e^{-i\theta} + q(x) e^{-2i\theta} \right] \right\} . \tag{9.23}$$

Now the Bloch low temperature law is $\Psi \propto y^4 \propto |z|^{-4}$ which indicates that the contribution to Ψ in (9.23) is of minor importance at very low temperatures.

The inference to be drawn from this result is that the dominant contribution to Ψ at very low temperatures is concealed in the residual series

$$\sum_{n=1}^{\infty} y^{2n}\left\{A_n(X)-\frac{K}{\sqrt{1-X^2}}(2n)!\,\rho^n(\cos\theta)^{2n+1}\left[\cos(2n+1)\theta+\frac{-p(X)\sin 2n\theta+q(X)\cos(2n-1)\theta}{2n}\right]\right\} \tag{9.24}$$

whose origin lies of course in the inexactitude of late-term formulae when applied also to early terms. To investigate this supposition, it is convenient once again to restrict further discussion to the special case X=0. (The theoretical conclusion (2.8) is that Ψ is independent of X in the low temperature limit.) Knowing the higher order coefficients given in (9.10), we can subtract out from the residual series (9.24) more of the terms which we know to be more slowly varying than $\sim y^4$ at low temperatures, so facilitating investigation of those which remain.

To determine the extreme low temperature behaviour, we therefore modify (9.12) for X=0 to

$$\Psi(0)=\sum_{n=0}^{\infty} y^{2n} A_0^n$$

$$= 1 + A_0^1 y^2 + K\sum_{n=2}^{\infty}\frac{(2n)!}{(-z_0^2)^n}\left[1+\frac{c}{2n}+\frac{d}{2n(2n-1)}+\frac{e}{2n(2n-1)(2n-2)}+\frac{f}{2n(2n-1)(2n-2)(2n-3)}\right]$$

$$+\sum_{n=2}^{\infty} y^{2n}\left\{A_0^n - K(2n)!\,\rho^n\left[1+\frac{c}{2n}+\frac{d}{2n(2n-1)}+\frac{e}{2n(2n-1)(2n-2)}+\frac{f}{2n(2n-1)(2n-2)(2n-3)}\right]\right\} \tag{9.25}$$

Invoking (9.13),

$$\sum_{n=2}^{\infty} \frac{(2n)!}{(-z_0^2)^n} = z_0 f(z_0) - 1 + \frac{2}{z_0^2} ,$$

$$\sum_{n=2}^{\infty} \frac{(2n-1)!}{(-z_0^2)^n} = - g(z_0) + \frac{1}{z_0^2} ,$$

$$\sum_{n=2}^{\infty} \frac{(2n-2)!}{(-z_0^2)^n} = - \frac{1}{z_0^2} \left[z_0 f(z_0) - 1 \right] , \tag{9.26}$$

$$\sum_{n=2}^{\infty} \frac{(2n-3)!}{(-z_0^2)^n} = \frac{1}{z_0^2} g(z_0) ,$$

$$\sum_{n=2}^{\infty} \frac{(2n-4)!}{(-z_0^2)^n} = \frac{1}{z_0^3} f(z_0) ,$$

none of which vary faster than $z_0^{-3} (\sim y^3)$ for small z_0 (large y). For $\Psi(0)$ to vary as $\sim y^4$ at low temperatures therefore, such variation must be contained in the residual series

$$\sum_{n=2}^{\infty} y^{2n} \left\{ A_0^n - K(2n)!\, \rho^n \left[1 + \frac{c}{2n} + \frac{d}{2n(2n-1)} + \frac{e}{2n(2n-1)(2n-2)} + \frac{f}{2n(2n-1)(2n-2)(2n-3)} \right] \right\} . \tag{9.27}$$

Table 9.2 lists for n between 2 and 12 the values of the coefficients A_0^n and of the residual coefficients of y^{2n} in (9.27) - i.e. those after subtracting from A_0^n our approximation for a late term. Although the latter are very much smaller than the former, the difference in order of magnitude increasing with n, it is clear that the series (9.27) is asymptotic. For $y \lesssim 3$, its approximate value may be obtained by truncating the series, adopting here the empirical procedure of including only <u>half</u> of the least term, known to produce accurate results for similar asymptotic series in which successive

n	A_0^n	Coeff. of y^{2n} in (9.27)
2	-0.216821×10^{-1}	0.234917×10^{-2}
3	0.239029×10^{-1}	-0.218816×10^{-3}
4	-0.439558×10^{-1}	0.448605×10^{-4}
5	0.130427×10^{0}	-0.167672×10^{-4}
6	-0.572084×10^{0}	0.160277×10^{-4}
7	0.347973×10^{1}	-0.337616×10^{-4}
8	-0.280223×10^{2}	0.120455×10^{-3}
9	0.288537×10^{3}	-0.630792×10^{-3}
10	-0.369711×10^{4}	0.450128×10^{-2}
11	0.576842×10^{5}	-0.418050×10^{-1}
12	-0.107664×10^{7}	0.489175×10^{0}

Table 9.2

terms alternate in sign. The error introduced may be roughly estimated by comparing the chosen value with the values corresponding to the retention of one extra or one fewer term in the series. The

y	$S(y)$	$S(y)/y^4$
1.0	0.002166 (5)	0.002166 (5)
1.2	0.00436 (2)	0.00210 (1)
1.4	0.00780 (9)	0.00203 (2)
1.6	0.0127 (1)	0.00194 (2)
1.8	0.0197 (5)	0.00188 (5)
2.0	0.029 (1)	0.00181 (6)
2.2	0.042 (1)	0.00179 (4)
2.4	0.057 (4)	0.00172 (12)
2.6	0.074 (13)	0.0016 (3)
2.8	0.09 (3)	0.0015 (5)
3.0	0.11 (7)	0.0014 (9)

Table 9.3

number of terms in the sum is 5 for $y \simeq 1$, dropping to 2 for $y \simeq 3$, this being the approximate upper limit of applicability. The resulting values of the sum (9.27) denoted by $S(y)$ are shown in Table 9.3 together with those of $S(y)/y^4$.

From the slow decrease of the figures in the last column it is evident that $S(y)$ varies in this range of y a little more slowly than $\sim y^4$; a graphical plot of $\log S$ versus $\log y$ reveals the approximate variation to be $\sim y^{3.75}$ over the region $1 \lesssim y \lesssim 3$ except possibly near $y = 3$ where $S(y)$ is rather uncertain anyway. The proximity of this to $\sim y^4$ is encouraging in view of the none-too-large values of y which have been employed.

It is also noteworthy that the general magnitude of $S(y)/y^4$ is of the same order as the theoretically expected value. For (2.8) predicts the variation of Ψ in the low temperature limit to be $\Psi \simeq \frac{1}{4}y^4/g_5(\infty) = 0.002009\, y^4$. It is true that the figures for $S(y)/y^4$ shown here suggest a limit (supposing that such a limit exists) considerably smaller than 0.002009. This is not unduly disturbing, however, since the data in Table 9.3 prove to be rather sensitive to the values assigned to the constants c, d, e, f etc. As remarked in the previous section, the absolute errors in the later coefficients are probably very much greater than indicated in (9.10). Their magnitude is difficult to estimate, but analysis of the effects caused by slightly adjusting c, d, and e to a different but mutually consistent set of values indicates that the absolute error in f may be of the same size as the quoted value for f itself. If we now argue that f is so unreliable that it may just as well be omitted, the same calculation as before but putting $f = 0$ yields a new table for $S(y)$ and $S(y)/y^4$ whose values are approximately 20% larger than those corresponding in Table 9.3. (This does not mean that uncertainties in these coefficients must affect our estimate of Ψ, since any change in the contribution $S(y)$ will be exactly compensated by an equal and opposite change in the value of the third term in (9.25)). Thus the evidence is that the extreme low temperature behaviour predicted by Bloch is indeed contained within the residual series.

Chapter 10

CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

A convenient point has now been reached for summarising the results achieved and suggesting the lines along which future work might profitably proceed.

The central core of the new method of solution to the Bloch equation is the expansion of the solution as a double series in rising powers of non-dimensional temperature and energy variables. Insertion into the original integral equation then leads to a recurrence relation for the two-index coefficients a_ℓ^n (if the independent variable x is selected) or A_ℓ^n (if the alternative variable X is preferred).

From then on, the complexity of the recurrence relation necessitates resort to approximate methods. The two techniques which may be employed to re-assemble the series are contained mainly in Chapter 7 and in Chapters 8 and 9 - for brevity, these will be called Methods I and II respectively. The main feature of Method I is the approximation of the coefficients a_ℓ^n by the similar set $\hat{a}_\ell^n$, without systematic investigation of the dependence of either on the indices n and ℓ ; this yields eventually the result (7.84) in which the required solution ψ is expressed in terms of the corresponding function $\hat{\psi}$. By contrast, Method II concentrates on finding the approximate functional form of the polynomials $\sum a_\ell^n x^\ell$ or $\sum A_\ell^n X^{2\ell}$, whose outcome for ψ or Ψ is (9.7) or its low temperature equivalent.

It should be emphasized that neither of Methods I and II has yet been developed to its full potential; ways of doing this are noted in the next few sections. Even though the analysis is incomplete, however, the results already obtained in Chapters 7, 8 and 9 show that the new technique displayed in this thesis for finding the solution to the Bloch equation is capable of yielding the functional form and numerical value of the solution at both high and low temperatures.

10.1 Extension of Method I

There are two ways in which the determination of the solution in Chapter 7 may be further improved. The first is to define yet another set of coefficients, $a^{\dagger n}_{\ell}$ say, which approximate a^{n}_{ℓ} even better than $\hat{a}^{n}_{\ell}$. The definition would be similar to that for $\hat{a}^{n}_{\ell}$ (see eq. (7.1)) except that the first two terms of the t-summation in (3.23) would be retained instead of just the first one. The corresponding function $\psi^{\dagger}$, defined by

$$\psi^{\dagger}(x) = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{2n} a^{\dagger n}_{\ell} \, x^{\ell} , \tag{10.1}$$

is the solution to a fourth order differential equation obtained from the infinite order differential equation (7.34) for ψ by retaining only the t =0, 1 and 2 terms in the summation over t. This equation may be solved by the method of successive approximations, but the analysis proves to be rather messy and the advantage obtained is probably small in proportion to the labour involved.

The other way involves the analytic study of the 'residual' series in (7.84):

$$\sum_{n=0}^{\infty} y^{2n} \left[\sum_{\ell=0}^{2n} a^{n}_{\ell} x^{\ell} - c q^{2n} \sum_{\ell=0}^{2n} \hat{a}^{n}_{\ell} x^{\ell} \right] . \tag{10.2}$$

Here the polynomials $\sum a^{n}_{\ell} x^{\ell}$ are identical to the corresponding polynomials $\sum A^{n}_{\ell} X^{2\ell}$ studied in Chapter 8. A similar analysis for $\sum \hat{a}^n_\ell x^\ell$ would enable the analytic form of the coefficients of y^{2n} to be determined, so enabling the summation over n to be carried out just as in Chapter 9. Since the coefficients $\hat{a}^n_\ell$ mimic the variation of a^n_ℓ with n and ℓ, it is highly likely that the polynomials $\sum \hat{a}^n_\ell x^\ell$ will prove to be of the same analytic form as $\sum a^n_\ell x^\ell$, but differ in the numerical values of the constants which occur. However although this procedure might well produce the most accurate answer possible at high temperatures, it is hardly likely to better Method II at low temperatures, since the $c\hat{\psi}$ constituent of (7.84) no longer contains the dominant contribution to ψ. (Recall the conclusion of § 7.6 that $\hat{\psi} \sim y^{-2}$ at low temperatures, contrasting with $\psi \sim y^4$.) Since the procedure for finding ψ by first calculating $\hat{\psi}$ is certainly more long-winded than the more direct route of Method II, and is likely to be superior to the latter only when the latter is perfectly adequate anyway (i.e. at high temperatures), we conclude that Method II is a more suitable candidate for further development than Method I.

10.2 Extension of Method II

The most obvious improvement to Method II as it stands would involve eliciting the terms of third and higher order for general values of X, not just for X = 0. This would be accomplished for $X < 1$ by first finding the corresponding terms for $X > 1$, following the pattern established in § 8.5 and § 8.6. Expanding the third order term $\gamma(X)$ as

$$\gamma(X) = \gamma_0 + \frac{\gamma_1}{X^2} + \frac{\gamma_2}{X^4} + \cdots, \qquad (10.3)$$

analogous to the expansion for $\beta(X)$ in (8.33), the coefficients γ_i may be found by a simple extension of the procedure for determining the coefficients β_i in (8.36) and (8.37), almost certainly with less accuracy due to the greater degree of cancellation involved. Whether it proves possible to fit $\gamma(X)$ to a formula constructed from individual terms such as those in (8.39) depends partly on how many terms and parameters there prove to be actually involved. The elucidation of $\beta(X)$ was rendered convincing in § 8.5 because the precisely evaluated coefficients β_0, β_1, β_2 ... comfortably outnumbered the parameters eventually found in $\beta(X)$; this happy state of affairs is unlikely to apply to the same extent with $\gamma(X)$, and the whole procedure could well break down if applied to the fourth order term $\delta(X)$.

If it transpires that further numerical analysis for general values of X is incapable of elucidating the higher order terms to the same extent and precision as for X = 0, it is still possible under such circumstances to improve the numerical evaluation of Ψ at high and moderate temperatures by the use of 'modifying factors', a technique devised by Dingle[53]. To illustrate its application to the best approximation for $A_n(X)$ so far found, we rewrite (9.1) in the form

$$A_n(X) = \frac{K}{\sqrt{1-X^2}}(2n)!\,\rho^n(\cos\theta)^{2n+1}\, b_n(X)\left\{\cos(2n+1)\theta + \frac{-P(X)\sin 2n\theta + q(X)\cos(2n-1)\theta}{2n}\right\}, \tag{10.4}$$

which constitutes the definition of the 'modifying factor' $b_n(X)$. Inclusion of this extra factor means that instead of (9.5) we are obliged to evaluate

$$\sum_{n=s}^{\infty} \frac{(2n)!}{(-z^2)^n}\, b_n(X). \tag{10.5}$$

For fixed X, $b_n(X)$ will obviously tend to unity as n increases through large values, so differences of these quantities will be small.

It is then advantageous to expand $b_n(X)$ by the Gregory 'backwards difference formula'

$$b_n = b_s + \frac{(n-s)}{1!}\nabla b_s + \frac{(n-s)(n-s+1)}{2!}\nabla^2 b_s + \cdots, \qquad (10.6)$$

where

$$\nabla b_s = b_s - b_{s-1}, \quad \nabla^2 b_s = \nabla b_s - \nabla b_{s-1}, \text{ etc.} \qquad (10.7)$$

This enables (10.5) to be evaluated eventually as

$$\sum_{n=s}^{\infty} \frac{(2n)!}{(-z^2)^n} b_n(X) = \frac{(2s)!}{(-z^2)^s} b_s(X) \Big[\Pi_{2s}(z) - $$

$$- z\, \Pi_{2s}^{(1)}(z) \frac{\nabla b_s(X)}{b_s(X)} + z^2\, \Pi_{2s}^{(2)}(z) \frac{\nabla^2 b_s(X)}{b_s(X)} + \cdots \Big], \qquad (10.8)$$

where $\Pi^{(1)}, \Pi^{(2)}, \ldots$ are reduced derivatives of Π. A similar expression holds for $\sum_{n=s}^{\infty}(2n-1)!\, b_n(X)/(-z^2)^n$ so the final result for Ψ in place of (9.7) is

$$\Psi(X) = \sum_{n=0}^{s-1} y^{2n} A_n(X) + \frac{K}{\sqrt{1-X^2}} \rho^s (2s)!\, y^{2s} (\cos\theta)^{2s+1} b_s(X)\, \mathcal{R}\, e^{(2s+1)i\theta} \times$$

$$\Big\{ \Big[\Pi_{2s}(z) + \frac{i\, p(X) e^{-i\theta} + q(X) e^{-2i\theta}}{2s} \Pi_{2s-1}(z) \Big] - z \frac{\nabla b_s(X)}{b_s(X)} \Big[\Pi_{2s}^{(1)}(z) + $$

$$+ \frac{i\, p(X) e^{-i\theta} + q(X) e^{-2i\theta}}{2s} \Pi_{2s-1}^{(1)}(z) \Big] + z^2 \frac{\nabla^2 b_s(X)}{b_s(X)} \Big[\Pi_{2s}^{(2)}(z) + \frac{i\, p(X) e^{-i\theta} + q(X) e^{-2i\theta}}{2s} \Pi_{2s-1}^{(2)}(z) \Big] + \cdots \Big\}.$$

$$(10.9)$$

Though obviously an improvement at high and moderate temperatures, this formula fails to provide much advantage at low temperatures, since s is then small and the sequence b_s, ∇b_s, $\nabla^2 b_s$, ... may not be uniformly decreasing in magnitude.

10.3 Generalisation to Impure and Non-Degenerate Metals

We now recall that two fairly drastic assumptions were incorporated into the Bloch integral equation at an early stage in our treatment: that the metal under scrutiny is completely degenerate ($\gamma = kT/\varsigma$ is zero) and completely pure ($\xi = 0$). Generalisation of the methods developed in this thesis to the case where neither assumption need be made is possible in principle but is accompanied by additional complexities of varying severity.

Extension to the case of an impure metal is reasonably straightforward, except that retention of the impurity term in (3.1) means that the solution ψ can no longer be an even function of y. The expansion of ψ as a double series in rising powers of y and x analogous to (3.7) must now include odd as well as even powers of y, and the recurrence relation developed for the coefficients will involve the parameter ξ in addition to the original parameter p. In all other respects there is no apparent reason why the analysis should not proceed exactly along the lines laid down for a pure metal.

Extension to the case of a non-degenerate metal is unfortunately much more complicated. To observe how the main difficulty arises, it is sufficient to consider Rhodes' first approximation (2.20) for a non-degenerate metal:

$$\phi_1(\eta) = \frac{\frac{1}{2} y^4 (1+\gamma\eta)^{3/2}}{\displaystyle\int_{-y}^{y} \frac{e^{\eta}+1}{e^{\eta+z}+1} \, \frac{z^4\,dz}{|1-e^{-z}|}} \quad . \tag{10.10}$$

As was noted at the begining of § 3.2, expansion of the R.H.S. of this expression omitting the $(1 + \gamma\eta)^{3/2}$ factor leads to a result of the same form (though with different coefficients) as was later found to represent the complete solution (for a completely degenerate metal). Retaining the $(1 + \gamma\eta)^{3/2}$ factor therefore and recalling the relation (6.3) between η and the preferred independent variable X, we see that the coefficients of the powers of y in the series expansion of the R.H.S. of (10.10) will no longer just be <u>polynomials</u> in X, but will be <u>infinite power series</u> in X; the same must obviously be true of the expansion representing the complete solution for ϕ or ϕ^*. It looks then as if extension of the theory to non-degenerate metals possesses new and possibly less pleasant features than were encountered for a degenerate metal, and no attempt has so far been made to develop the theory in this direction.

10.4 <u>Evaluation of the Electrical Conductivity</u>

The main purpose of this work was not so much to evaluate the transport coefficients of interest as to elucidate the analytic form of the distribution function from which such coefficients are derived. Since in addition the second order effects such as thermal conductivity depend on non-zero powers of γ being retained in the Bloch equation, it is inappropriate to attempt anything more than a brief discussion of how the electrical conductivity might be evaluated for a perfectly pure metal.

The electrical conductivity was originally stated to be determined by the transport integral K_1 defined by (1.25); after the numerous subsequent transformations, simplifications and changes of variable, this is found to be proportional to $\int_0^1 \Psi(x)dx$, the coefficient of proportionality being displayed in (3.8). Direct integration of any of the final forms for Ψ - eq.(9.7) for example- is hardly practicable. Probably the best technique is simply to integrate the polynomials appearing in the exact expansion of the function Ψ :

$$\int_0^1 \Psi(X)\,dX = \int_0^1 dX \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{n} A_\ell^n X^{2\ell} = \sum_{n=0}^{\infty} y^{2n} \sum_{\ell=0}^{n} \frac{A_\ell^n}{2\ell+1} \,. \tag{10.11}$$

The single - index coefficients $\sum_{\ell=0}^{n} A_\ell^n / (2\ell+1)$ may now be evaluated and analysed to discover their dependence on n, enabling the summation over n to be carried out by a method appropriate to the temperature range under consideration - analogous to the procedure demonstrated in § 9.1 or § 9.2.

10.5 The Problem of Polar Semiconductors

As remarked towards the end of Chapter 2, the Boltzmann equation for polar semiconductors reduces to a difference equation instead of to an integral equation due to the assumption of a single frequency ν_0 for the dominant phonon optical mode. The other physical assumptions are similar to those for metals, and it is interesting to see if the method of solution developed for the latter can also be applied to polar semiconductors.

Just as for metals, care must be exercised in selecting the most appropriate formulation of the equation whose solution is desired. Starting from the difference equation for each of the two formal relaxation times $\tau(\eta)$ and $\tau^*(\eta)$ (see for example Durney[45]) it is easy to show that in the limit of complete degeneracy τ^* is proportional to τ, the difference equation for τ being

$$g^{1/2} = \frac{e^y}{e^y-1}\,\frac{e^\eta+1}{e^{\eta+y}+1}\left[(\alpha+\tfrac{1}{2})\,\tau(\eta) - \alpha\,\tau(\eta+y)\right]$$

$$+ \frac{1}{e^y-1}\,\frac{e^\eta+1}{e^{\eta-y}+1}\left[(\alpha+\tfrac{1}{2})\,\tau(\eta) - \alpha\,\tau(\eta-y)\right], \tag{10.12}$$

with

$$g = \frac{\varsigma}{h\nu_0} \;, \quad \alpha = \ln 2 g^{1/2} - \tfrac{1}{2} \;,$$
$$\eta = \frac{E - \varsigma}{kT} \;, \quad y = \frac{h\nu_0}{kT} \;. \tag{10.13}$$

From a glance at this equation, it is evident that $\tau(\eta)$ is primarily a function of e^{η} and of e^{y} rather than of η and y , which makes it appropriate to select the new variables

$$X = \frac{e^{\eta} - 1}{e^{\eta} + 1} \;, \qquad Y = \frac{e^{y} - 1}{e^{y} + 1} \;. \tag{10.14}$$

Defining a new dependent variable Ψ by

$$\tau(\eta) = g^{1/2} \frac{2Y}{1 - Y^2} \Psi(X) \;, \tag{10.15}$$

the difference equation satisfied by Ψ is found to be

$$1 - X^2Y^2 = (2\alpha + 1)\Psi(X) - \alpha(1 - XY)\Psi\left(\frac{X+Y}{1+XY}\right) - \alpha(1 + XY)\Psi\left(\frac{X-Y}{1-XY}\right). \tag{10.16}$$

The first order approximation to $\Psi(X)$ at high temperatures, analogous to Rhodes' first approximation to $\phi(\eta)$ for metals, is obtained by setting $Y = 0$ in the argument of Ψ but leaving all other quantities unaltered. This yields

$$\Psi_1(X) = 1 - X^2Y^2 \;. \tag{10.17}$$

Correction terms $\Psi_2(X)$, $\Psi_3(X)$ ... may be determined by the method of successive approximations, examination of which reveals the probable form of the expansion of $\Psi(X)$ as an infinite series in rising powers of Y . As part of a research project directed along these lines, Christie[52] has shown that the correct expansion is

$$\Psi(X) = \sum_{n=0}^{\infty} Y^{2n} \sum_{\ell=0}^{n} d_\ell^n X^{2\ell}, \tag{10.18}$$

of exactly the same form as (6.6). Substituting in (10.16), expanding in rising powers of Y and X and equating coefficients of equal powers on the two sides of the equation, a recurrence relation is readily obtained for the coefficients d_ℓ^n. After the evaluation of the first several dozen of these by digital computer, numerical analysis analogous to that in Chapter 8 may be carried out to reveal the approximate form of the polynomials $\sum d_\ell^n X^{2\ell}$. Although this has not yet been carried through to completion, the startling result has emerged that the first order approximation to these polynomials is identical in form to that of the polynomials $\sum A_\ell^n X^{2\ell}$ discussed in Chapter 8. Thus

$$\sum_{\substack{\ell=0 \\ (X>1)}}^{n} d_\ell^n X^{2\ell} = \frac{K'}{\sqrt{X^2-1}} \frac{(2n)!\left(\frac{\pi}{2}\sqrt{-\rho'}\right)^{2n}}{\left[\tanh^{-1}(1/X)\right]^{2n+1}} \left\{ 1 + O\left(\tfrac{1}{n}\right) \right\}, \tag{10.19}$$

$$\sum_{\substack{\ell=0 \\ (X<1)}}^{n} d_\ell^n X^{2\ell} = \frac{4K'}{\pi\sqrt{1-X^2}} (2n)!\, \rho'^{n} (\cos\theta)^{2n+1} \left\{ \cos(2n+1)\theta + O\left(\tfrac{1}{n}\right) \right\}, \tag{10.20}$$

where ρ' and K' are constants and θ is defined in (8.22); hence the same mathematical functions must be involved in the two physical problems. This result, for which no explanation is immediately forthcoming, implies automatic advantages in respect of the straightforward application of the methods of Chapter 9 to the problem of calculating the function Ψ ; it also demonstrates how the twin problems of transport in metals and in polar semiconductors are more closely connected than would be revealed by simply comparing the integral and difference equations in terms of which they are formulated.

Appendix 1

SUMMATIONS INVOLVING STIRLING NUMBERS OF THE SECOND KIND

In this appendix we derive various summation relations involving Stirling numbers of the second kind. These relations were quoted and applied in Chapters 3, 6 and 7, but do not appear to be generally known. We also discuss why other summations encountered in these chapters apparently do not sum to simple and convenient forms.

A1.1 Starting from the well known relation

$$\sum_{\ell=\nu}^{\infty} \frac{\nu!}{\ell!} C_\ell^\nu z^\ell = (e^z - 1)^\nu, \tag{A1.1}$$

we differentiate with respect to z, yielding

$$\begin{aligned}\sum_{\ell=\nu}^{\infty} \frac{\nu!}{\ell!} C_\ell^\nu \ell z^{\ell-1} &= \nu e^z (e^z-1)^{\nu-1} \\ &= \frac{\nu}{z}(e^z-1)^\nu\left(\frac{-z}{e^{-z}-1}\right) \\ &= \frac{\nu}{z}\sum_{m=\nu}^{\infty} \frac{\nu!}{m!} C_m^\nu z^m \sum_{r=0}^{\infty} \frac{B_r}{r!}(-1)^r z^r \\ &= \nu \sum_{\ell=\nu}^{\infty} \frac{z^{\ell-1}}{\ell!} \sum_{m=\nu}^{\ell} \nu! \binom{\ell}{m} C_m^\nu B_{\ell-m} (-1)^{\ell-m}.\end{aligned} \tag{A1.2}$$

Equating coefficients of $z^{\ell-1}$,

$$\sum_{m=\nu}^{\ell} \binom{\ell}{m}(-1)^m B_{\ell-m}\, C_m^{\nu} = (-1)^{\ell}\, \frac{\ell}{\nu}\, C_{\ell}^{\nu} \quad , \quad \nu \neq 0 . \tag{A1.3}$$

Similarly,

$$\begin{aligned}\sum_{\ell=\nu-1}^{\infty} \frac{(\nu-1)!}{\ell!}\, C_{\ell}^{\nu-1} z^{\ell} &= (e^{z}-1)^{\nu-1} \\ &= \frac{(e^{z}-1)^{\nu}}{z}\,\frac{z}{e^{z}-1} \\ &= \frac{1}{z}\sum_{m=\nu}^{\infty} \frac{\nu!}{m!}\, C_m^{\nu} z^{m} \sum_{r=0}^{\infty} \frac{B_r}{r!} z^{r} \\ &= \sum_{\ell=\nu}^{\infty} \frac{z^{\ell-1}}{\ell!} \sum_{m=\nu}^{\ell} \nu! \binom{\ell}{m} C_m^{\nu} B_{\ell-m} .\end{aligned} \tag{A1.4}$$

Equating coefficients of $z^{\ell-1}$,

$$\sum_{m=\nu}^{\ell} \binom{\ell}{m} B_{\ell-m}\, C_m^{\nu} = \frac{\ell}{\nu}\, C_{\ell-1}^{\nu-1} \quad , \quad \nu \neq 0 . \tag{A1.5}$$

A1.2 Consider the quantity

$$I = \sum_{\nu=r}^{s+r} \frac{1}{\nu} \binom{s}{\nu-r} (e^{-z}-1)^{\nu} . \tag{A1.6}$$

This may be expanded as an infinite series in rising powers of z in two distinct ways, arising from different treatments of the $(e^{-z}-1)^{\nu}$

factor. Firstly,

$$I = \sum_{\nu=r}^{s+r} \frac{1}{\nu} \binom{s}{\nu-r} \sum_{n=\nu}^{\infty} z^n (-1)^n \frac{\nu!}{n!} C_n^\nu$$

$$= \sum_{n=r}^{\infty} \frac{z^n (-1)^n}{n!} \sum_{\nu=r}^{s+r,\, n} (\nu-1)! \binom{s}{\nu-r} C_n^\nu \; . \tag{A1.7}$$

On the other hand,

$$(e^{-z}-1)^\nu = \frac{(1-e^z)^\nu}{(e^z)^\nu} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{m=0}^{n} C_n^m \left(\frac{d}{dy}\right)^m \frac{(1-y)^\nu}{y^\nu}\Big|_{y=1}$$

$$= \sum_{n=\nu}^{\infty} \frac{z^n}{n!} \sum_{m=\nu}^{n} C_n^m (m-1)! (-1)^m \nu \binom{m}{\nu} \; . \tag{A1.8}$$

Hence

$$I = \sum_{\nu=r}^{s+r} \frac{1}{\nu} \binom{s}{\nu-r} \sum_{n=\nu}^{\infty} \frac{z^n}{n!} \sum_{m=\nu}^{n} C_n^m (m-1)! (-1)^m \nu \binom{m}{\nu}$$

$$= \sum_{n=r}^{\infty} \frac{z^n}{n!} \sum_{m=r}^{n} C_n^m (m-1)! (-1)^m \sum_{\nu=r}^{s+r,\, m} \binom{s}{\nu-r} \binom{m}{\nu}$$

$$= \sum_{n=r}^{\infty} \frac{z^n}{n!} \sum_{m=r}^{n} C_n^m (m-1)! (-1)^m \binom{m+s}{r+s} \; . \tag{A1.9}$$

Combining (A1.7) and (A1.9),

$$\sum_{\nu=r}^{n} C_n^{\nu}(\nu-1)!(-1)^{\nu}\binom{\nu+s}{r+s} = (-1)^n \sum_{\nu=r}^{s+r,n} (\nu-1)!\binom{s}{\nu-r} C_n^{\nu} . \tag{A1.10}$$

When s = 0 we have the special case

$$\sum_{\nu=r}^{n} C_n^{\nu}(\nu-1)!(-1)^{\nu}\binom{\nu}{r} = (-1)^n(r-1)!\, C_n^{r} . \tag{A1.11}$$

We can now identify the obstacle to summing either side of (A1.10) for $s \neq 0$. Each side is proportional to the coefficient of z^n in the expansion of the function I and this will be of simple form only if I is a reasonably simple function of z. We first rewrite (A1.6) as

$$I = (e^{-z}-1)^r \sum_{\nu=0}^{s} \frac{1}{\nu+r} \binom{s}{\nu}(e^{-z}-1)^{\nu} . \tag{A1.12}$$

The troublesome $(\nu + r)^{-1}$ factor is best expanded as a Newton series:

$$\frac{1}{\nu+r} = \frac{1}{r} + \binom{\nu}{1}\Delta\left(\frac{1}{r}\right) + \binom{\nu}{2}\Delta^2\left(\frac{1}{r}\right) + \cdots = (r-1)!\sum_{m=0}^{\nu} \frac{\nu!}{(\nu-m)!}\,\frac{(-1)^m}{(r+m)!} . \tag{A1.13}$$

Hence

$$\begin{aligned} I &= (r-1)!(e^{-z}-1)^r \sum_{m=0}^{s} \frac{(-1)^m}{(r+m)!} \sum_{\nu=m}^{s} \binom{s}{\nu}\frac{\nu!}{(\nu-m)!}(e^{-z}-1)^{\nu} \\ &= (r-1)!\,(e^{-z}-1)^r e^{-sz} \frac{s!}{(r+s)!} \sum_{m=0}^{s} (-1)^m \binom{r+s}{s-m}(1-e^{z})^m \\ &= (-1)^s(r-1)!(e^{-z}-1)^{r+s} \frac{s!}{(r+s)!} \sum_{\ell=0}^{s} (-1)^{\ell}\binom{r+s}{\ell}\frac{1}{(1-e^{z})^{\ell}} . \end{aligned} \tag{A1.14}$$

The sum over ℓ is a truncated binomial series which is related to the hypergeometric function $F(a\ ,\ b\ ;\ c\ ;\ x)$ in the following way (See Erdélyi et al.[34], p.101):

$$\sum_{\ell=0}^{s} \binom{r+s}{\ell} \frac{1}{(e^{z}-1)^{\ell}} = \binom{r+s}{s} \frac{1}{(e^{z}-1)^{s}}\, F(-s,\ 1\ ;\ r+1\ ;\ 1-e^{z}). \tag{A1.15}$$

Hence

$$I = \frac{1}{r}\left(e^{-z}-1\right)^{r} e^{-sz}\, F\left(-s,\ 1\ ;\ r+1\ ;\ 1-e^{z}\right). \tag{A1.16}$$

The transformation properties of the hypergeometric function allow this equation to be written in many different ways. However none of them is any simpler than (A1.16) and none will allow the coefficient of z^{n} to be extracted in any simpler form than is given by either side of (A1.10). This is excepting the special case $s = 0$: the function I is then just

$$I_{s=0} = \frac{1}{r}\left(e^{-z}-1\right)^{r}, \tag{A1.17}$$

which is responsible for the simplicity of (A1.11).

A1.3 Starting from (A1.11), we multiply both sides by $\left[-\frac{1}{2}(1+X)\right]^{r}$ and sum over r from 1 to n:

$$(-1)^{n}\sum_{r=1}^{n}(r-1)!\, C_{n}^{r}(-1)^{r}\left(\frac{1+X}{2}\right)^{r} = \sum_{r=1}^{n}(-1)^{r}\left(\frac{1+X}{2}\right)^{r}\sum_{\nu=r}^{n} C_{n}^{\nu}(\nu-1)!\,(-1)^{\nu}\binom{\nu}{r}$$

$$= \sum_{\nu=1}^{n} C_n^{\nu} (\nu-1)! (-1)^{\nu} \sum_{r=1}^{\nu} (-1)^r \left(\frac{1+X}{2}\right)^r \binom{\nu}{r}$$

$$= \sum_{\nu=1}^{n} C_n^{\nu} (\nu-1)! (-1)^{\nu} \left[\left(\frac{1-X}{2}\right)^{\nu} - 1\right].$$

(A1.18)

Putting $X = 1$, we deduce the well known relation *

$$\sum_{\nu=1}^{n} C_n^{\nu} (\nu-1)! (-1)^{\nu} = 0 , \qquad \text{(A1.19)}$$

whence

$$(-1)^n \sum_{\nu=1}^{n} (\nu-1)! C_n^{\nu} (-1)^{\nu} \left(\frac{1+X}{2}\right)^{\nu} = \sum_{\nu=1}^{n} C_n^{\nu} (\nu-1)! (-1)^{\nu} \left(\frac{1-X}{2}\right)^{\nu}. \qquad \text{(A1.20)}$$

Expanding each side in rising powers of X,

$$(-1)^n \sum_{q=0}^{n} X^q \sum_{\nu=q,1}^{n} (\nu-1)! C_n^{\nu} (-\tfrac{1}{2})^{\nu} \binom{\nu}{q} = \sum_{q=0}^{n} (-X)^q \sum_{\nu=q,1}^{n} (\nu-1)! C_n^{\nu} (-\tfrac{1}{2})^{\nu} \binom{\nu}{q}$$

(A1.21)

from which there follows

$$\sum_{\nu=q}^{n} (\nu-1)! \; C_n^{\nu} (-\tfrac{1}{2})^{\nu} \binom{\nu}{q} = 0 , \quad n+q \text{ odd}. \qquad \text{(A1.22)}$$

A1.4 It was stated in Chapter 6 that it does not appear possible to express either of the following two summations in more concise form:

* Strictly, this deduction can only be made for even values of n. But the result is true for all n, e.g. see ref. 30, p.189.

$$J = \sum_{\nu=2r}^{2t} (\nu-1)!\left(-\tfrac{1}{2}\right)^{\nu} C_{2t}^{\nu} \binom{\nu}{2r}, \qquad \text{(A1.23)}$$

$$K = \sum_{\nu=|2r|}^{2t} (\nu-1)!\left(-\tfrac{1}{2}\right)^{\nu} C_{2t}^{\nu} \sum_{m=0,-2r}^{2\ell-2r,\nu,\nu-2r} (-1)^{m}\binom{\nu}{m+2r}\binom{\nu}{m}\binom{2\ell-2r+\nu-m}{\nu}. \qquad \text{(A1.24)}$$

To justify this, we first investigate the summation over ν. Since (A1.23) is a special case of (A1.24) with ℓ = r and r positive, it is sufficient to show that (A1.23) is intractable.

It follows from (A1.1) that C_{2t}^{ν} is equal to $(2t)!/\nu!$ times the coefficient of z^{2t} in the expansion of $(e^{z} - 1)^{\nu}$. Thus

$$J = \sum_{\nu=2r}^{2t} (\nu-1)!\left(-\tfrac{1}{2}\right)^{\nu}\binom{\nu}{2r}\frac{(2t)!}{\nu!}\,\frac{1}{2\pi i}\oint_{u=0}\frac{(e^{u}-1)^{\nu}\,du}{u^{2t+1}}$$

$$= \frac{(2t)!}{2\pi i}\oint_{u=0}\frac{du}{u^{2t+1}}\sum_{\nu=2r}^{\infty}\frac{1}{\nu}\binom{\nu}{2r}\left(\frac{1-e^{u}}{2}\right)^{\nu}$$

$$= \frac{(2t)!}{2r\;\;2\pi i}\oint_{u=0}\frac{du}{u^{2t+1}}\sum_{\nu=2r-1}^{\infty}\binom{\nu}{2r-1}\left(\frac{1-e^{u}}{2}\right)^{\nu+1}$$

$$= \frac{(2t)!}{2r\;\;2\pi i}\oint_{u=0}\frac{du}{u^{2t+1}}\left[\tanh\frac{u}{2}\right]^{2r}, \qquad \text{(A1.25)}$$

where the path of integration is round a small circle enclosing the origin in the complex u-plane. We require therefore the coefficient of u^{2t} in the expansion of $(\tanh u/2)^{2r}$ in rising powers of u. Unfortunately this quantity cannot be expressed in any simpler form than that originally given in (A1.23).

Turning attention to the summation over m in (A1.24), it is possible to express this in terms of the generalised hypergeometric function ${}_3F_2$ defined by Erdélyi et al.[34], p.182:

$$ {}_3F_2\left[\begin{matrix} a_1, a_2, a_3 ; z \\ \rho_1, \rho_2 \end{matrix}\right] = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n (a_3)_n}{(\rho_1)_n (\rho_2)_n} \frac{z^n}{n!} \qquad \text{(A1.26)} $$

where, as usual,

$$ \begin{aligned} (a)_n &= a(a+1)\dots(a+n-1) \\ &= \frac{(a+n-1)!}{(a-1)!} \quad , \ a \text{ positive} , \\ &= (-1)^n \frac{(-a)!}{(-a-n)!} \quad , \ a \text{ negative}. \end{aligned} \qquad \text{(A1.27)} $$

With these definitions,

$$ \sum_m (-1)^m \binom{\nu}{m+2r} \binom{\nu}{m} \binom{2\ell-2r+\nu-m}{\nu} = $$

$$ = \sum_m \frac{(-1)^m \ \nu! \ \ \nu! \ (2\ell-2r+\nu-m)!}{(m+2r)!(\nu-m-2r)! \, m! \, (\nu-m)! \, \nu! (2\ell-2r-m)!} $$

$$ = \frac{(2\ell-2r+\nu)!}{(2r)!(\nu-2r)!(2\ell-2r)!} \sum_{m=0}^{\infty} \frac{(2r-\nu)_m (-\nu)_m (2r-2\ell)_m (-1)^m}{(-2\ell+2r-\nu)_m (2r+1)_m \ m!} $$

$$ = \binom{\nu}{2r} \binom{2\ell-2r+\nu}{\nu} {}_3F_2 \left[\begin{matrix} 2r-\nu, -\nu, 2r-2\ell ; -1 \\ -2\ell+2r-\nu, 2r+1 \end{matrix}\right]. \qquad \text{(A1.28)} $$

However the generalised hypergeometric function is in this case neither Saalschützian nor well poised. (For definitions of these terms, see Ref.34, p.188). This means that it is very unlikely to be summable unless it can be reduced to one of the few known special cases, which does not appear to be possible.

Another general method for summing products of binomial coefficients involves expressing the summation as an integral representation:

$$\sum_{m} (-1)^m \binom{\nu}{m+2r}\binom{\nu}{m}\binom{2\ell-2r+\nu-m}{\nu} =$$

$$= \frac{1}{(2\pi i)^3} \sum_{m=0}^{\infty} \oint\oint\oint \frac{dx\, dy\, dz\, (1+x)^{\nu}(1+y)^{\nu}(1+z)^{-1-\nu}}{x^{m+2r+1}\; y^{m+1}\; z^{2\ell-2r-m+1}}$$

$$= \frac{1}{(2\pi i)^3} \oint\oint\oint \frac{dx\, dy\, dz\, (1+x)^{\nu}(1+y)^{\nu}(1+z)^{-1-\nu}}{x^{2r+1}\left(y-\frac{z}{x}\right) z^{2\ell-2r+1}}$$

$$= \frac{1}{(2\pi i)^2} \oint\oint \frac{dx\, dz\, (1+x)^{\nu}(x+z)^{\nu}(1+z)^{-1-\nu}}{x^{2r+\nu+1}\; z^{2\ell-2r+1}} .$$

(A1.29)

This cannot be further developed without expanding terms in the numerator, which effectively reverses the order of the argument.

A1.5 Finally, we derive a relation which is needed in § 7.3.

$$\sum_{n=m+p}^{\infty} z^n \frac{(m+p)!}{n!} C_n^{m+p} = (e^z-1)^{m+p}$$

$$= \sum_{t=m}^{\infty} z^t \frac{m!}{t!} C_t^m \sum_{r=p}^{\infty} z^r \frac{p!}{r!} C_r^p$$

$$= \sum_{n=m+p}^{\infty} \frac{z^n}{n!} \sum_{t=m}^{n-p} \binom{n}{t} m!\, C_t^m\, p!\, C_{n-t}^p \, .$$

(A1.30)

Equating coefficients of powers of z,

$$\sum_{t=m}^{n-p} \binom{n}{t} C_t^m \, C_{n-t}^p = \binom{m+p}{p} C_n^{m+p} \, . \tag{A1.31}$$

This result may be extended by the following argument.

$$\sum_{t=m}^{n-p} \binom{n}{t}(n-t)\, C_t^m \, C_{n-t}^p = n\binom{m+p}{p} C_n^{m+p} - n \sum_{t=m}^{n-p} \binom{n-1}{t-1} C_t^m \, C_{n-t}^p \, . \tag{A1.32}$$

Now

$$\sum_{t=m}^{n-p} \binom{n-1}{t-1} C_t^m \, C_{n-t}^p = \sum_{t=m-1}^{n-p-1} \binom{n-1}{t} C_{t+1}^m \, C_{n-t-1}^p$$

$$= \sum_{t=m-1}^{n-p-1} \binom{n-1}{t} \left(C_t^{m-1} + m\, C_t^m \right) C_{n-t-1}^p$$

$$= \binom{m-1+p}{p} C_{n-1}^{m-1+p} + m \sum_{t=m}^{n-p-1} \binom{n-1}{t} C_t^m \, C_{n-1-t}^p$$

$$= \binom{m-1+p}{p} C^{m-1+p}_{n-1} + m \binom{m+p}{p} C^{m+p}_{n-1}$$

$$= \binom{m+p-1}{p} C^{m+p}_{n} \quad .$$

$$\tag{A1.33}$$

Hence, combining (A1.32) and (A1.33),

$$\sum_{t=m}^{n-p} \binom{n}{t}(n-t)\, C^{m}_{t}\, C^{p}_{n-t} = n \binom{m+p-1}{p-1} C^{m+p}_{n} \quad . \tag{A1.34}$$

Appendix 2

SOME REMARKS ON THE COMPUTATIONAL PROBLEMS INVOLVED

The initial computational task was to calculate successive coefficients a_ℓ^n from the recurrence relation (3.23) and, later, the coefficients A_ℓ^n from the corresponding relation (6.19). After calculation, each set of numbers was stored in punched card form, the card deck being used as data for subsequent investigation of the form of a_ℓ^n (or A_ℓ^n) and the calculation and analysis of the associated polynomials.

Apart from simple algebraic functions, the recurrence relations involve binomial coefficients, Stirling numbers of the second kind and Bernoulli numbers. These are best computed in separate subprogrammes at the beginning of the main programme and are thereafter available for insertion in the main calculation.

In the first subprogramme, the binomial coefficients are generated by successive applications of the simple recurrence relation

$$\binom{i}{j} = \binom{i-1}{j} + \binom{i-1}{j-1}, \tag{A2.1}$$

with obvious modifications at the end points $j = 0$ and $j = i$. Reference to either (3.23) or (6.19) shows that the Stirling numbers C_{2i}^j always occur multiplied by the factor $(j-1)!/(2i-1)!$, so it is convenient to compute the array of numbers

$$D_i^j = \frac{(j-1)!}{(2i-1)!} C_{2i}^j \tag{A2.2}$$

instead of the Stirling numbers themselves. The latter satisfy a recurrence relation

$$C_n^m = C_n^{m-1} + m\, C_{n-1}^m , \tag{A2.3}$$

and the recurrence relation generating the D_i^j is easily proved to be

$$D_i^j = \frac{1}{(2i-1)(2i-2)} \left[(j-1)(j-2)\, D_{i-1}^{j-2} + (j-1)(2j-1)\, D_{i-1}^{j-1} + j^2\, D_{i-1}^{j} \right]. \tag{A2.4}$$

For given i , j runs from 1 to $2i$. The special cases of (A2.4) at the end points are

$$D_i^1 = \frac{D_{i-1}^1}{(2i-1)(2i-2)} , \tag{A2.5}$$

$$D_i^2 = \frac{3\, D_{i-1}^1 + 4\, D_{i-1}^2}{(2i-1)(2i-2)} , \tag{A2.6}$$

$$D_i^{2i-1} = i , \tag{A2.7}$$

$$D_i^{2i} = 1 . \tag{A2.8}$$

A second subprogramme has been developed to compute the array of numbers D_i^j by successive application of these relations.

By the convention established in Chapter 3, D_i^j is taken to mean $B_{2i}/(2i)!$ when $j = 0$, where B_n is the n'th Bernoulli number. This set of numbers ($i = 0, 1, \ldots$) is tabulated in standard reference tables and is best entered directly into the programme as a set of constants.

Part Two

THE ELECTRICAL CONDUCTIVITY OF A THIN METAL FILM IN A LONGITUDINAL MAGNETIC FIELD

SUMMARY OF PART TWO

As for Part One, it is convenient to summarise the development of the argument chapter by chapter.

Chapter 11 The Boltzmann equation is solved for thin film geometry under the following assumptions:

(a) A relaxation time $\tau(\underline{k})$ exists.

(b) Electrons are quasi-free ($\underline{k} = m^* \underline{v}/\hbar$ where m^* is the effective mass).

(c) Scattering of electrons at the boundary is wholly diffuse.

The electric current density is then evaluated, leading to an expression for the electrical conductivity σ involving a triple integral. In the "high-field" region $d/2r_0 \geqslant 1$ (d = thickness of film, r_0 = cyclotron radius), the limits of integration permit evaluation of all three integrations, yielding σ in terms of elementary functions. For smaller fields however ($d/2r_0 < 1$), only one of the integrations can be carried out, and the final expression for σ involves four functions denoted by A, B, C and D; the first three are expressed as single integrals and the fourth as a double integral. The problem is now to devise methods for expressing these approximately in terms of known functions.

Chapter 12 Each of the integrals A, B, C and D is a function of the two parameters $\theta_0 = \sin^{-1}(d/2r_0)$ and $\kappa = d/\ell$ (ℓ is the bulk mean free path), and the magnitude of each determines the most appropriate method of calculation. The interesting values of κ lie in the range $0.01 \lesssim \kappa \lesssim 1$ so that for a large range of κ, θ_0 values, $\mu = \kappa/2\sin\theta_0 \lesssim 1$. It is then convenient to expand the exponential appearing in each integral in rising powers of μ and integrate term by term.

Chapter 13 For sufficiently small θ_0, μ becomes large and the resulting predominance of the exponential term allows the integrals A, B and C to be expressed as asymptotic series. Though intended primarily for the range $\mu \gtrsim 1$, these series are servicable also for $\mu \lesssim 1$, though with less accuracy. The exponent in the integrand of D exhibits different behaviour as $\theta_0 \to 0$ compared with those in A, B and C, and a Taylor expansion in descending powers of μ yields the most suitable approximation.

Chapter 14 Here the conductivity calculated by the methods described in chapters 12 and 13 is compared with the corresponding value found by Kao[22] by direct numerical integration. Close agreement is obtained between the two results, except for a few small ranges of the two parameters involved.

The theory is also compared with the limited range of experimental results so far available. Unfortunately experiments on thin films, compared with those on wires, have not been very numerous. Of those which have been reported, some are unsuitable as a test of the theory because the metal does not comply with one or more of the conditions implicit in the theory, e.g. that the Fermi surface shall be spherical. Theoretically, the best metals for experimental observation of the effect would be the alkali or noble metals. The experimental results of Gaidukow and Kadletsova[51] probably constitute the most convincing evidence, imperfect though it is, for the existence of the effect analysed in this thesis.

Chapter 11

THIN FILM IN A LONGITUDINAL MAGNETIC FIELD

11.1 Solution to the Boltzmann Equation

Consider a thin film lying between the planes $y = 0$ and $y = d$. We assume that the electrons are quasi-free with effective mass m^*. A magnetic field H and an electric field E are applied in the z direction. Let

$$N(\underline{v}, y)\, dx\, dy\, dz\, dv_x\, dv_y\, dv_z$$

be the number of electrons in the volume element $dx\,dy\,dz$ with velocities in the range v_x and $v_x + dv_x$, ...; N is to be determined from the Boltzmann equation

$$\frac{\partial N}{\partial y} v_y + \frac{\partial N}{\partial \underline{v}} \cdot \dot{\underline{v}} = - \frac{N - N_0}{\tau}, \tag{11.1}$$

where τ is the relaxation time and N_0 the equilibrium Fermi-distribution. Since

$$-e\left(\underline{E} + \frac{1}{c}\, \underline{v} \times \underline{H}\right) = m^* \dot{\underline{v}},$$

we get

$$\frac{\partial N}{\partial y} v_y - \frac{e}{m^*}\left[E \frac{\partial N}{\partial v_z} + \frac{H}{c}\left(v_y \frac{\partial N}{\partial v_x} - v_x \frac{\partial N}{\partial v_y}\right)\right] = - \frac{N - N_0}{\tau}. \tag{11.2}$$

When E and H are zero, N must be the equilibrium function N_0. Hence $\partial N_0/\partial y = 0$, i.e. N_0 is not a function of position. Putting $N - N_0 = n(\underline{v}, y)$ and replacing N by N_0 in the term involving E, we have as a very good approximation

$$\frac{\partial n}{\partial y} v_y - \frac{e}{m^*}\left[E \frac{\partial N_0}{\partial v_z} + \frac{H}{c}\left(v_y \frac{\partial N}{\partial v_x} - v_x \frac{\partial N}{\partial v_y}\right)\right] = -\frac{n}{\tau}. \tag{11.3}$$

Since $N_0 = N_0(v_x^2 + v_y^2 + v_z^2)$, this reduces to

$$\frac{\partial n}{\partial y} v_y - \frac{e}{m^*}\left[E \frac{\partial N_0}{\partial v} \frac{v_z}{v} + \frac{H}{c}\left(v_y \frac{\partial n}{\partial v_x} - v_x \frac{\partial n}{\partial v_y}\right)\right] = -\frac{n}{\tau}. \tag{11.4}$$

Putting

$$n(\underline{v}, z) = \frac{eE\tau}{m^*} \frac{\partial N_0}{\partial v} \frac{v_z}{v}\left[1 + g(v_x, v_y, y)\right], \tag{11.5}$$

we obtain

$$v_y \frac{\partial g}{\partial y} - \alpha\left(v_y \frac{\partial g}{\partial v_x} - v_x \frac{\partial g}{\partial v_y}\right) + \frac{g}{\tau} = 0, \tag{11.6}$$

where $\alpha = eH/m^*c$.

Let us now transform to spherical polar coordinates in velocity space:

$$v_z = v\cos\theta, \quad v_x = v\sin\theta\cos\phi, \quad v_y = v\sin\theta\sin\phi.$$

Then (11.6) becomes

$$v\sin\theta\sin\phi \frac{\partial g}{\partial y} + \alpha \frac{\partial g}{\partial \phi} + \frac{g}{\tau} = 0. \tag{11.7}$$

The subsidiary equations for solving this equation are

$$\frac{dy}{v \sin\theta \sin\phi} = \frac{d\phi}{\alpha} = -\tau \frac{dg}{g}, \qquad (11.8)$$

of which two independent solutions are

$$g \propto \exp(-\phi/\alpha\tau) \quad \text{and} \quad \cos\phi + \frac{\alpha y}{v \sin\theta} = \text{const.}$$

The general solution is therefore

$$g = -\exp\left\{-\frac{1}{\alpha\tau}\left[\phi + \Omega\left(\cos\phi + \frac{\alpha y}{v\sin\theta}\right)\right]\right\} \qquad (11.9)$$

where Ω is an arbitrary function which may include v and θ as parameters.

We assume that electron scattering at the boundary is wholly diffuse, which implies that n = 0 for those electrons which are moving away from the boundary just after collision. Thus $g = -1$ for $y = 0$, $v_y > 0$ and also for $y = d$, $v_y < 0$. These conditions yield

$$g = -\exp\left[-\frac{1}{\alpha\tau}\left(\phi - \cos^{-1}\varepsilon_1\right)\right], \quad v_y > 0,$$

$$g = -\exp\left[-\frac{1}{\alpha\tau}\left(\phi - 2\pi + \cos^{-1}\varepsilon_2\right)\right], \quad v_y < 0, \qquad (11.10)$$

where

$$\varepsilon_1 = \cos\phi + \frac{\alpha y}{v \sin\theta}, \qquad \varepsilon_2 = \cos\phi + \frac{\alpha(y-d)}{v\sin\theta}.$$

However these equations can only be true provided $|\varepsilon_1|, |\varepsilon_2| \leqslant 1$.

Geometrical considerations to be discussed in the next section show that the complete solution is:

(a) For $v_y > 0 (0 < \phi \leqslant \pi)$:

$$
\begin{aligned}
g &= -\exp\left[-\frac{1}{\alpha\tau}\left(\phi - \cos^{-1}\varepsilon_1\right)\right], \quad \varepsilon_1 < 1 \\
&= -\exp\left[-\frac{1}{\alpha\tau}\left(\phi + \cos^{-1}\varepsilon_2\right)\right], \quad \varepsilon_1 \geqslant 1, \ \varepsilon_2 > -1 \\
&= 0, \quad \varepsilon_1 \geqslant 1, \ \varepsilon_2 \leqslant -1;
\end{aligned}
\tag{11.11}
$$

(b) For $v_y < 0 (\pi < \phi \leqslant 2\pi)$:

$$
\begin{aligned}
g &= -\exp\left[-\frac{1}{\alpha\tau}\left(\phi - 2\pi + \cos^{-1}\varepsilon_2\right)\right], \quad \varepsilon_2 > -1 \\
&= -\exp\left[-\frac{1}{\alpha\tau}\left(\phi - \cos^{-1}\varepsilon_1\right)\right], \quad \varepsilon_2 \leqslant -1, \ \varepsilon_1 < 1 \\
&= 0, \quad \varepsilon_2 \leqslant -1, \ \varepsilon_1 \geqslant 1.
\end{aligned}
\tag{11.12}
$$

11.2 Calculation of the Conductivity

Writing the solution obtained above in the compact form $g = -\exp(-\Psi/\alpha\tau)$ where Ψ appears in full in (11.11) and (11.12), the current density in the z-direction is

$$
\begin{aligned}
j &= -e\iiint v_z \, n(\underline{v}, y)\, dv_x\, dv_y\, dv_z \\
&= -\frac{e^2 E}{m^*}\int_0^\infty dv\, \tau\, v^3 \frac{\partial N_0}{\partial v}\int_0^\pi d\theta \cos^2\theta \sin\theta \int_0^{2\pi} d\phi \left(1 - e^{-\Psi/\alpha\tau}\right).
\end{aligned}
\tag{11.13}
$$

Averaging the current density over the cross-section and expressing the resultant effective conductivity $\sigma = \bar{j}/E$ as a fraction of the bulk conductivity σ_0 ,

$$\frac{\sigma}{\sigma_0} = \frac{3}{4\pi d}\int_0^d dy \int_0^{\pi} d\theta \cos^2\theta \sin\theta \int_0^{2\pi} d\phi \left(1 - e^{-\Psi/\alpha\tau}\right)$$

$$= 1 - \frac{3}{4\pi d}\int_0^d dy \int_0^{\pi} d\theta \cos^2\theta \sin\theta \int_0^{2\pi} d\phi \, e^{-\Psi/\alpha\tau} . \qquad (11.14)$$

The geometrical interpretation of Ψ is as follows: Under the influence of the magnetic field in the z-direction, the trajectory of an electron travelling at an angle θ to the z-axis is a helix whose projection on the x - y plane is a circle of radius $r = r_0 \sin\theta$ where $r_0 = m^* vc/eH$ is the cyclotron radius. Then since $\cos\phi + \alpha y/v \sin\theta = \cos\phi + y/r$, $\phi - \cos^{-1}\varepsilon_1$ is the angle (Ψ) traversed round this circle by an electron moving between a point on the surface y = 0 and a general point in the interior of the metal at which the instantaneous direction of motion is θ , ϕ ,see fig. 1.

Similarly when $0 < \phi \leqslant \pi$, $\phi + \cos^{-1}\varepsilon_2$ is the angle traversed since an electron collided with the surface y = d. The significance of the inequalities in (11.11) is that, for an electron currently travelling with positive v_y, the surface y = 0 was the one last involved in a collision if $\varepsilon_1 < 1$. If $\varepsilon_1 \geqslant 1$, but $\varepsilon_2 > -1$, the previous trajectory last intersected the surface y = d and avoided collision with the other surface. If $\varepsilon_1 \geqslant 1$ and $\varepsilon_2 \leqslant -1$, however, the previous trajectory involved collisions with neither surface ($\Psi = \infty$) and the out-of-balance term $n(\underline{v}, y)$ in the distribution function is the same as that in the bulk metal, for this combination of θ , ϕ , y values. A similar argument holds for (11.12), for those electrons currently moving with negative v_y. Hence the interpretation of (11.14) is that $\sigma - \sigma_0$ depends purely on the reduction in free path of those electrons whose trajectories intersect the bounding surface.

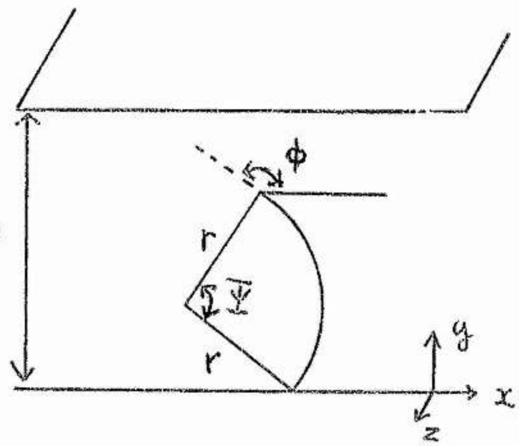


Fig. 1 The electron orbit projected on the x-y plane.

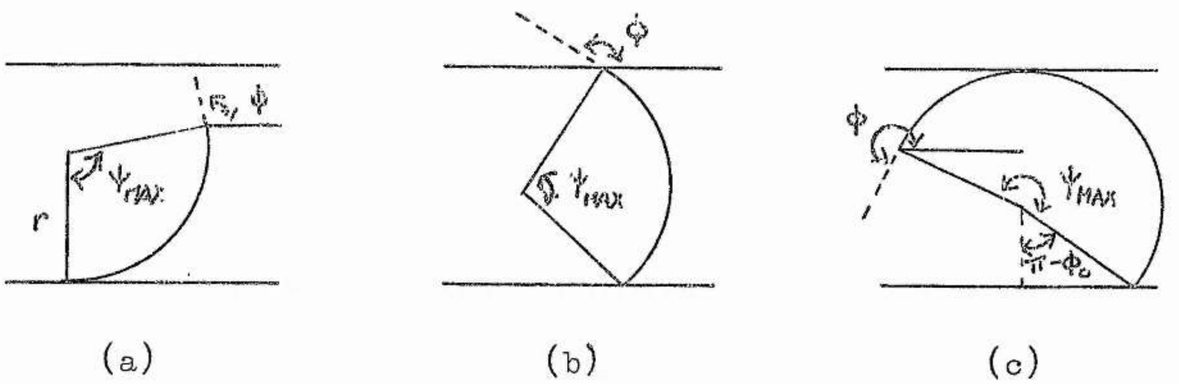


Fig. 2 Projected orbits corresponding to the maximum possible value for ψ for given values of θ and ϕ, when $\theta_0 < \theta < \pi/2$ and ϕ lies in the ranges (a) 0 to ϕ_0, (b) ϕ_0 to π, (c) π to $\pi + \phi_0$.

This is the formal justification for Chambers' kinetic theory approach.[10,11]

By symmetry, the two surfaces contribute equally to the decrease in the conductivity and for convenience we write

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{2\pi d}\int_0^d dy \int_0^\pi d\theta \cos^2\theta \sin\theta \int_0^{2\pi} d\phi \, e^{-\psi/\alpha\tau} , \qquad (11.15)$$

where

$$\begin{aligned} \psi &= \phi - \cos^{-1}\varepsilon_1 , \quad \varepsilon_1 < 1 \\ &= \infty , \quad \varepsilon_1 \geqslant 1 ; \end{aligned} \qquad (11.16)$$

i.e. we now consider only those orbits originating from the surface $y = 0$. Now $(\alpha\tau)^{-1} = m^*c/eH\tau = r_0/\ell = \mu$, say, ℓ being the mean free path. Changing the variable from y to ψ and noting that $\psi(y,\theta,\phi) = \psi(y,-\theta,\phi)$,

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3r_0}{\pi d}\int_0^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{2\pi} d\phi \int d\psi \sin(\phi-\psi)\, e^{-\mu\psi} . \qquad (11.17)$$

Here, the upper limit of 2π for ϕ is applicable only if no trajectory which would otherwise contribute to the integral in (11.17) is disallowed by virtue of its previous intersection with the other surface, this being the case when $d \geqslant 2r_0$. The limits for ψ in (11.17) are then 0 and ϕ for $0 \leqslant \phi \leqslant \pi$ and $2(\phi - \pi)$ and ϕ for $\pi \leqslant \phi \leqslant 2\pi$. The integrals in (11.17) are then elementary, yielding

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{16K}\,\frac{1 + 8\mu^2 - e^{-2\pi\mu}}{1 + 4\mu^2} , \quad d \geqslant 2r_0 , \qquad (11.18)$$

where $K = d/\ell$, the result previously obtained by Koenigsberg,[15] Azbel[16] and Barron and McDonald.[21]

When d $< 2r_0$, define $\sin\theta_0 = d/2r_0$.. For $0 \leq \theta \leq \theta_0$ $(2r \leq d)$ collisions with the upper surface again do not occur, but when $\theta_0 < \theta \leq \pi/2$ $(2r > d)$ the upper limits for ψ are reduced due to the impossibility of an electron trajectory lying partly outside the film. Defining $\phi_0 = \cos^{-1}(1 - d/r) = \cos^{-1}(1 - 2\sin\theta_0/\sin\theta)$, the limits for the ψ -integration in (11.17) are as follows:
For $0 \leq \theta \leq \theta_0$:

$$0 \text{ and } \phi \quad , \quad 0 \leq \phi \leq \pi ,$$
$$2(\phi-\pi) \text{ and } \phi \quad , \quad \pi \leq \phi \leq 2\pi .$$

For $\theta_0 < \theta \leq \pi/2$ (see fig. 2):

$$0 \text{ and } \phi \quad , \quad 0 \leq \phi \leq \phi_0 ,$$
$$0 \text{ and } \phi - \cos^{-1}(\cos\phi + d/r) , \quad \phi_0 \leq \phi \leq \pi ,$$
$$2(\phi-\pi) \text{ and } \phi + \phi_0 - \pi \quad , \quad \pi \leq \phi \leq \pi + \phi_0 ,$$

the maximum allowed value of ϕ being $\pi + \phi_0$.

Hence, performing the integration over ψ and as much of the integration over ϕ and θ as is possible in closed form, (11.17) reduces to

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3}{32\pi K} \frac{2\pi(1+8\mu^2) - e^{-2\pi\mu}(4\theta_0 - \sin 4\theta_0)}{1+4\mu^2}$$
$$- \frac{3}{\pi K}\left[\frac{1}{4\mu^2+1}\left(A_2 - 2\sin\theta_0 B_2 + 4\mu\sin^{\frac{1}{2}}\theta_0 C_2\right) - \right.$$
$$\left. - \frac{2}{\mu^2+1}\left(A - \sin\theta_0 B + \mu\sin^{\frac{1}{2}}\theta_0 C\right)\right] - \frac{3D}{2\pi\sin\theta_0(\mu^2+1)} \quad , \quad d < 2r_0 \tag{11.19}$$

where

$$A = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \, e^{-\mu\phi_0} , \tag{11.20}$$

$$B = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin\theta \, e^{-\mu\phi_0} , \tag{11.21}$$

$$C = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin\theta \, (\sin\theta - \sin\theta_0)^{1/2} e^{-\mu\phi_0} , \tag{11.22}$$

$$D = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_{\phi_0}^{\pi} d\phi \left[u - \mu(1-u^2)^{1/2} \right] e^{-\mu(\phi - \cos^{-1}u)} , \tag{11.23}$$

$$u(\theta,\phi) = \cos\phi + 2\sin\theta_0 / \sin\theta , \tag{11.24}$$

and where the subscript 2 denotes that μ in (11.20)-(11.22) is to be replaced by 2μ.

It is worth remarking that as $\theta_0 \to 0$, A, B and C all vanish and (11.19) reduces to

$$\begin{aligned} \frac{\sigma}{\sigma_0} &= 1 - \frac{3}{8K} + \frac{3}{\pi K} \int_0^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{\pi} d\phi \sin\phi \, \exp(-K/\sin\theta\sin\phi) \\ &= 1 - \frac{3}{8K} + \frac{3}{4\pi K} \int_0^{\pi} d\theta \cos^2\theta \sin^2\theta \int_0^{2\pi} d\phi \, |\sin\phi| \exp(-K/\sin\theta|\sin\phi|) \end{aligned} \tag{11.25}$$

The transformation $\cos\theta = \sin\theta' \cos\phi'$, $\sin\theta \sin\phi = \cos\theta'$ with $\sin\theta \; d\theta \; d\phi$ replaced by $\sin\theta' \; d\theta' \; d\phi'$ leads immediately to the expression for the conductivity of a thin film in the absence of a magnetic field found by Fuchs[8].

Chapter 12

EVALUATION OF THE INTEGRALS A, B, C AND D FOR $\mu \lesssim 1$

12.1 Evaluation of A

Considering first the integral A, we rewrite (11.20)as

$$A = e^{-\mu\pi} \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \exp\left[2\mu \sin^{-1}(1 - \sin\theta_0/\sin\theta)^{1/2}\right]$$

$$= e^{-\mu\pi} \sum_{m=0}^{\infty} \frac{(2\mu)^m}{m!} Z_m \qquad (12.1)$$

where

$$Z_m = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \left[\sin^{-1}(1 - \sin\theta_0/\sin\theta)^{1/2}\right]^m . \qquad (12.2)$$

Expansion of the $\sin^{-1}$ term in rising powers of $(1 - \sin\theta_0/\sin\theta)^{1/2}$ yields

$$Z_0 = \Upsilon_0 ,$$

$$Z_1 = \Upsilon_{\frac{1}{2}} + \frac{1}{6}\Upsilon_{\frac{3}{2}} + \frac{3}{40}\Upsilon_{\frac{5}{2}} + \frac{5}{112}\Upsilon_{\frac{7}{2}} + \frac{35}{1152}\Upsilon_{\frac{9}{2}} + \cdots ,$$

$$Z_2 = \Upsilon_1 + \frac{1}{3}\Upsilon_2 + \frac{8}{45}\Upsilon_3 + \frac{4}{35}\Upsilon_4 + \frac{128}{1575}\Upsilon_5 + \cdots ,$$

$$Z_3 = \Upsilon_{\frac{3}{2}} + \frac{1}{2}\Upsilon_{\frac{5}{2}} + \frac{111}{360}\Upsilon_{\frac{7}{2}} + \frac{3229}{15120}\Upsilon_{\frac{9}{2}} + \cdots ,$$

$$Z_4 = \gamma_2 + \frac{2}{3}\gamma_3 + \frac{7}{15}\gamma_4 + \frac{328}{945}\gamma_5 + \cdots,$$

$$Z_5 = \gamma_{\frac{5}{2}} + \frac{5}{6}\gamma_{\frac{7}{2}} + \frac{47}{72}\gamma_{\frac{9}{2}} + \cdots,$$

$$Z_6 = \gamma_3 + \gamma_4 + \frac{39}{45}\gamma_5 + \cdots,$$

$$Z_7 = \gamma_{\frac{7}{2}} + \frac{7}{6}\gamma_{\frac{9}{2}} + \cdots,$$

$$Z_8 = \gamma_4 + \frac{4}{3}\gamma_5 + \cdots,$$

$$Z_9 = \gamma_{\frac{9}{2}} + \cdots, \tag{12.3}$$

where

$$\gamma_p = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \left(1 - \sin\theta_0/\sin\theta\right)^p. \tag{12.4}$$

When p is an integer, the calculation of γ_p is elementary, while the γ_p of half-integer order may be exactly expressed in terms of tabulated elliptic integrals. Thus

$$\gamma_{\frac{1}{2}} = h\Big[\left(-24s + 20s^2 - 10s^3 - 15s^4\right)K + \left(-20s - 20s^2 + 15s^3 + 15s^4\right)E$$
$$+ \left(48 - 24s^2 + 15s^4\right)\beta\Big],$$

$$\gamma_{3/2} = h\Big[\left(-24s + 84s^2 + 6s^3 + 9s^4\right)K + \left(-84s - 84s^2 - 9s^3 - 9s^4\right)E$$
$$+ \left(48 + 72s^2 - 9s^4\right)\beta\Big],$$

$$\gamma_{5/2} = h\Big[\left(-24s + 148s^2 - 266s^3 - 15s^4\right)K + \left(-148s - 148s^2 + 15s^3 + 15s^4\right)E$$
$$+ \left(48 + 360s^2 + 15s^4\right)\beta\Big],$$

$$\tau_{7/2} = h\Big[\left(-24s + 212s^2 - 1210s^3 - 663s^4\right)K \; +$$

$$+ \left(-212s - 212s^2 + 663s^3 + 663s^4\right)E \; + \left(48 + 840s^2 - 105s^4\right)\beta\Big],$$

$$\tau_{9/2} = h\Big[\left(-24s + 276s^2 - 3210s^3 - 2639s^4 + 256s^5\right)K$$

$$+ \left(-276s - 276s^2 + 2639s^3 + 2639s^4\right)E \; + \left(48 + 1512s^2 - 945s^4\right)\beta\Big],$$

$$\tau_{11/2} = \text{----},$$

$$(12.5)$$

where $s = \sin\theta_0$, $h = (1 + s)^{-\frac{1}{2}}/192$, K and E are complete elliptic integrals of the first and second kind respectively, each of argument $k_1 = [(1 - s)/(1 + s)]^{1/2}$, and $\beta = (\pi/2)(1 + s)^{\frac{1}{2}}\Lambda_0(\pi/4, k_1)$ where Λ_0 is Heumann's lambda-function. - For definitions, see ref. 38, pp. 9, 10 and 35; tables are listed in refs. 23 and38.

12.2 Evaluation of B

The integral B differs from A only by a factor $\sin\theta$ in the integrand, and the method of calculation is similar. Thus

$$B = e^{-\mu\pi}\sum_{m=0}^{\infty}\frac{(2\mu)^m}{m!}Y_m \qquad (12.6)$$

where

$$Y_m = \int_{\theta_0}^{\pi/2} d\theta\,\cos^2\theta\,\sin\theta\left[\sin^{-1}\left(1 - \sin\theta_0/\sin\theta\right)^{1/2}\right]^m. \qquad (12.7)$$

When m = 1, (12.7) may be related to tabulated elliptic integrals without approximation. A preliminary integration by parts yields

$$Y_1 = \frac{1}{6}\sin^{\frac{1}{2}}\theta_0 \int_{\theta_0}^{\pi/2} \frac{\cos^4\theta \, d\theta}{\sin\theta(\sin\theta - \sin\theta_0)^{1/2}}, \tag{12.8}$$

which may be reduced to

$$Y_1 = \frac{\pi}{6}\left[1 - \Lambda_0(\theta_1, k_2)\right] + \frac{(2s)^{1/2}}{45}\left[(18 - s - 4s^2)K - (21 - 8s^2)E\right], \tag{12.9}$$

where $K = K(k_2)$, $E = E(k_2)$, $k_2 = \left[(1 - s)/2\right]^{1/2}$ and $\theta_1 =$ $= \sin^{-1}\left[2s/(1 + s)\right]^{\frac{1}{2}}$. For other values of m, Y_m is given by the R.H.S. of (12.3) with r_p replaced everywhere by

$$s_p = \int_{\theta_0}^{\pi/2} d\theta \, \cos^2\theta \, \sin\theta \, (1 - \sin\theta_0/\sin\theta)^p. \tag{12.10}$$

When p is an integer, s_p is again elementary, while for p =(integer+$\frac{1}{2}$) we have

$$s_{\frac{1}{2}} = h\Big[(-64s - 16s^2 - 24s^3)K + (64 + 64s + 24s^2 + 24s^3)E$$
$$+ (-96s + 24s^3)\beta\Big],$$

$$s_{3/2} = h\Big[(-64s + 272s^2 + 24s^3)K + (64 + 64s - 24s^2 - 24s^3)E$$
$$+ (-288s - 24s^3)\beta\Big],$$

$$s_{5/2} = h\Big[(-64s + 944s^2 + 648s^3)K + (64 + 64s - 648s^2 - 648s^3)E$$
$$+ (-480s + 120s^3)\beta\Big],$$

$$S_{7/2} = h\Big[(-64s + 2000s^2 + 1976s^3 - 256s^4)K$$

$$+ (64 + 64s - 1976s^2 - 1976s^3)E \ + (-672s + 840s^3)\beta\Big],$$

$$S_{9/2} = \frac{h}{5}\Big[(-320s + 17200s^2 + 20424s^3 - 6144s^4 - 768s^5)K$$

$$+ (320 + 320s - 20424s^2 - 20424s^3 + 768s^4 + 768s^5)E$$

$$+ (-4320s + 12600s^3)\beta\Big],$$

$$S_{11/2} = ----, \tag{12.11}$$

where

$$E = E(k_1), \quad K = K(k_1).$$

12.3 Evaluation of C

Treating the integral C in the same way as for A andB,

$$C = e^{-\mu\pi}\sum_{m=0}^{\infty}\frac{(2\mu)^m}{m!}X_m \quad , \tag{12.12}$$

where

$$X_m = \int_{\theta_0}^{\pi/2} d\theta\cos^2\theta\sin\theta\,(\sin\theta - \sin\theta_0)^{1/2}\Big[\sin^{-1}(1 - \sin\theta_0/\sin\theta)^{1/2}\Big]^m. \tag{12.13}$$

Expanding the $\sin^{-1}$ term, X_m is given by the R.H.S. of (12.3) with r_p replaced everywhere by

$$t_p = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^{3/2}\theta \left(1 - \sin\theta_0/\sin\theta\right)^{p+\frac{1}{2}} . \tag{12.14}$$

When p is an integer, this may be reduced to

$$t_0 = \frac{2^{3/2}}{105}\left[(5+8s-s^2-4s^3)K + (-16s+8s^3)E \right],$$

$$t_1 = \frac{2^{3/2}}{105}\left[(5+29s+27s^2+3s^3)K + (-58s-6s^3)E \right],$$

$$t_2 = \frac{2^{1/2}}{105}\left[(10+100s+180s^2-120s^3)K + (-200s+30s^3)E - 105s^3\gamma \right],$$

$$t_3 = \frac{2^{-\frac{1}{2}}}{105}\left[(20+284s+752s^2-1192s^3-210s^4)K + (-568s+914s^3)E - 735s^3\gamma \right],$$

$$t_4 = \frac{2^{-5/2}}{105}\left[(80+1472s+5136s^2-13056s^3-3990s^4+420s^5)K + (-2944s+12882s^3)E + (-6615s^3+420s^5)\gamma \right],$$

$$t_5 = \cdots\cdots , \tag{12.15}$$

where $E = E(k_2)$, $K = K(k_2)$ and $\gamma = \pi(2s)^{-\frac{1}{2}}\left[1 - \Lambda_0(\theta_1, k_2)\right]$.
When p = (integer + $\frac{1}{2}$), we find similarly

$$t_{1/2} = \frac{2^{3/2}}{105}\left[(5+21s)F - 42sE + (10+6s^2)\delta \right],$$

$$t_{3/2} = \frac{2^{3/2}}{105}\left[(5+42s+35s^2)F - 84sE + (10-8s^2)\delta \right],$$

$$t_{5/2} = \frac{2^{3/2}}{105}\Big[(5+63s+105s^2-105s^3)F + (-126s+210s^3)E + (10-162s^2)\delta\Big],$$

$$t_{7/2} = \frac{2^{3/2}}{105}\Big[(5+84s+210s^2-420s^3-35s^4)F + (-168s+840s^3)E + (10-526s^2)\delta\Big],$$

$$t_{9/2} = \frac{2^{3/2}}{105}\Big[(5+105s+350s^2-1050s^3-175s^4+21s^5)F$$

$$+ (-210s+2100s^3-42s^5)E + (10-1156s^2+42s^4)\delta\Big],$$

$$t_{11/2} = \cdots\cdots ,$$

(12.16)

where F and E are the incomplete elliptic integrals $F(\theta_2, 1/\sqrt{2})$ and $E(\theta_2, 1/\sqrt{2})$, $\theta_2 = \sin^{-1}(1-s)^{1/2}$, and $\delta = \left[\frac{1}{2}s(1-s^2)\right]^{1/2}$.

12.4 Evaluation of D

Considering now the integral D, we change to the new variable $\phi' = \frac{1}{2}(\pi - \phi)$ and drop the dashes immediately, whereupon (11.23) becomes

$$D = 2e^{-\mu\pi}\int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{q} d\phi \left[1-2g-2\mu(g-g^2)^{1/2}\right]\exp\left[2\mu(\phi+\sin^{-1}g^{1/2})\right],$$

(12.17)

where $q = \sin^{-1}(1-\sin\theta_0/\sin\theta)^{1/2}$ and $g = \sin^2 q - \sin^2\phi$.
Expanding the exponential in rising powers of μ and writing

$$D = 2e^{-\mu\pi} \sum_{m=0}^{\infty} D_m \mu^m , \tag{12.18}$$

where D_m is independent of μ, we obtain

$$D_0 = \int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{q} d\phi \, (1-2g) = 2\sin\theta_0 \, Y_1 - \sin^{1/2}\theta_0 \, X_0 \, . \tag{12.19}$$

The next coefficient is

$$D_1 = 2\int_{\theta_0}^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{q} d\phi \left[(1-2g)(\phi + \sin^{-1} g^{1/2}) - (g-g^2)^{1/2} \right] . \tag{12.20}$$

Expanding $\sin^{-1} g^{1/2}$ and $(g - g^2)^{1/2}$ in rising powers of $g^{1/2}$,

$$(1-2g)(\phi + \sin^{-1} g^{1/2}) - (g-g^2)^{1/2} = (1-2g)\phi - \frac{4}{3} g^{3/2} \left(1 + \frac{1}{10} g + \frac{9}{280} g^2 + \cdots \right). \tag{12.21}$$

Now

$$\begin{aligned} g &= \sin^2 q - \sin^2\phi \\ &= (q^2-\phi^2)\left[1 - \tfrac{1}{3}(q^2+\phi^2) + \tfrac{2}{45}(q^4+q^2\phi^2+\phi^4) - \tfrac{1}{315}(q^6+q^4\phi^2+q^2\phi^4+\phi^6) + \cdots \right] \end{aligned} \tag{12.22}$$

$$\therefore \quad g^{3/2}\left(1 + \frac{1}{10} g + \frac{9}{280} g^2 + \cdots \right) =$$

$$= (q^2-\phi^2)^{3/2} \left[1 - \frac{1}{5}(2q^2+3\phi^2) + \frac{1}{210}(12q^4 + 18q^2\phi^2 + 47\phi^4) + \cdots \right] . \tag{12.23}$$

Integration over ϕ may now be performed, yielding eventually

$$D_1 = 2\sin\theta_0 Y_2 - 2\sin^{1/2}\theta_0 X_1 + Z_0 - \sin\theta_0 Y_0 - \frac{\pi}{2}\left(Z_4 - \frac{1}{2}Z_6 + \frac{41}{480}Z_8 + \cdots\right). \tag{12.24}$$

Carrying out similar calculations for D_2 and D_3 , we find

$$D_2 = -\frac{2}{3}Z_3 - \frac{32}{15}Z_5 + \frac{88}{63}Z_7 - \frac{544}{2025}Z_9 + \cdots, \tag{12.25}$$

$$D_3 = -\left(\frac{\pi}{2}+\frac{2}{3}\right)Z_4 - \left(\frac{\pi}{12}+\frac{4}{9}\right)Z_6 + \left(\frac{53\pi}{320}+\frac{22}{45}\right)Z_8 + \cdots \tag{12.26}$$

The series (12.3) for Z_m and the corresponding series for X_m and Y_m converge rapidly when m is small, the convergence deteriorating as m increases. For a given number of terms included in the summation, a more accurate estimate of the value of these integrals may be obtained by applying the nonlinear e_1 transformation (e.g. Shanks[32]): for Y_1 , whose value is known exactly from (12.9), retention of the first 5 terms in the appropriate series gives a result accurate to 0.03% when $\theta_0 = 20^\circ$, compared with an accuracy of 0.15% without application of the transform. The various series in rising powers of μ such as in eqs. (12.1) and (12.18) are rapidly convergent for $\mu \lesssim 1$, particularly for θ_0 close to $\pi/2$. The series in (12.24) - (12.26) converge well for $0.5 \lesssim \sin\theta_0 \lesssim 1$; though less speedily convergent for $\sin\theta_0 \lesssim 0.5$, their applicability may again be extended by employing the e_1 transform.

Chapter 13

EVALUATION OF THE INTEGRALS A, B, C AND D FOR $\mu \gtrsim 1$

Substituting $\sin\theta_0/\sin\theta = \sin^2\chi$ in (11.20),

$$A = 2\sin^6\chi_0 \int_{\chi_0}^{\pi/2} d\chi \, \frac{\cos\chi}{\sin^9\chi} \left(\sin^4\chi - \sin^4\chi_0\right)^{1/2} e^{-2\mu\chi}, \tag{13.1}$$

where $\sin^2\chi_0 = \sin\theta_0$. An asymptotic series may be obtained for A by expanding all factors in the integrand except the exponential in rising powers of $(\chi - \chi_0)$ with the upper limit of integration replaced by ∞ (which can at most introduce an exponentially small error). However, the first few terms decrease rapidly only for $\mu >> 1$ which is the case here only for very small values of θ_0 . This is because $(\sin\chi)^{-9}$ varies at least as rapidly as $\exp(-2\mu\chi)$ in the important part of the integration range i.e. $\chi \sim \chi_0$. A series which is computationally useful for a much wider range of μ values may be found by first writing

$$(\sin\chi)^{-9} = e^{-9\log\sin\chi} = \frac{e^{-9(\chi-\chi_0)\cot\chi_0}}{\sin^9\chi_0}\left[1 + \tfrac{9}{2}(\chi-\chi_0)^2(\nu^2+1) - \right.$$

$$\left. - 3(\chi-\chi_0)^3(\nu^3+\nu) + \tfrac{1}{8}(\chi-\chi_0)^4(99\nu^4 + 186\nu^2 + 87) + \cdots\cdot\right], \tag{13.2}$$

where $\nu = \cot\chi_0$. Expanding the other factors except the exponential in rising powers of $(\chi - \chi_0)$, combining and integrating with the top limit of integration replaced by ∞ ,

$$A = \frac{2\pi^{1/2}\,\nu^{3/2}\,e^{-2\mu\chi_0}}{(2\mu+9\nu)^{3/2}}\Big[\,1 + \frac{3}{8}\,\frac{3\nu-5\nu^{-1}}{2\mu+9\nu} + \frac{5}{128}\,\frac{453\nu^2+250+21\nu^{-2}}{(2\mu+9\nu)^2}$$

$$+ \frac{105}{1024}\,\frac{43\nu^3-807\nu-591\nu^{-1}+3\nu^{-3}}{(2\mu+9\nu)^3}$$

$$+ \frac{21}{32768}\,\frac{1024335\nu^4+1576860\nu^2+758074+82140\nu^{-2}+495\nu^{-4}}{(2\mu+9\nu)^4} + \cdots\Big]. \qquad (13.3)$$

The versatility of this expansion may be judged from the fact that even taking the limiting case $\mu = 0$ when integral A reduces to Z_0 of the previous chapter, (13.3) yields a result to within 3% of the exact value of this integral for small values of θ_0.

The corresponding asymptotic series for B and C are

$$B = 2\sin^4\chi_0\int_{\chi_0}^{\pi/2} d\chi\,\frac{\cos\chi}{\sin^7\chi}\,(\sin^4\chi-\sin^4\chi_0)^{1/2}\,e^{-2\mu\chi}$$

$$= \frac{2\pi^{1/2}\,\nu^{3/2}\,e^{-2\mu\chi_0}}{(2\mu+7\nu)^{3/2}}\Big[\,1 + \frac{3}{8}\,\frac{3\nu-5\nu^{-1}}{2\mu+7\nu} + \frac{5}{128}\,\frac{357\nu^2+154+21\nu^{-2}}{(2\mu+7\nu)^2}$$

$$+ \frac{35}{1024}\,\frac{97\nu^3-1973\nu-1293\nu^{-1}+9\nu^{-3}}{(2\mu+7\nu)^3}$$

$$+ \frac{21}{32768}\,\frac{635535\nu^4+901980\nu^2+451834+61980\nu^{-2}+495\nu^{-4}}{(2\mu+7\nu)^4} + \cdots\Big], \qquad (13.4)$$

$$C = 2 \sin^5\chi_0 \int_{\chi_0}^{\pi/2} d\chi \, \frac{\cos^2\chi}{\sin^8\chi} \left(\sin^4\chi - \sin^4\chi_0\right)^{1/2} e^{-2\mu\chi}$$

$$= \frac{2\pi^{1/2}\cos\chi_0 \, \nu^{3/2} e^{-2\mu\chi_0}}{(2\mu + 8\nu)^{3/2}} \Bigg[1 + \frac{3}{8}\,\frac{3\nu - 9\nu^{-1}}{2\mu + 8\nu} + \frac{5}{128}\,\frac{405\nu^2 + 82 + 141\nu^{-2}}{(2\mu + 8\nu)^2}$$

$$+ \frac{35}{1024}\,\frac{113\nu^3 - 3961\nu - 2037\nu^{-1} - 75\nu^{-3}}{(2\mu + 8\nu)^3}$$

$$+ \frac{21}{32768}\,\frac{818415\nu^4 + 994860\nu^2 + 1039114 + 410700\nu^{-2} - 1665\nu^{-4}}{(2\mu + 8\nu)^4} + \cdots \Bigg]. \qquad (13.5)$$

The exponent in the integrand of integral D shows different behaviour as $\theta_0 \to 0$ from that of integrals A, B and C, tending as it does towards $(-\kappa/\sin\theta \, \sin\phi)$ instead of increasing without limit. Since κ is usually rather small, an adaptation of the theory given above for A, B and C is not immediately possible. It is important on the other hand to obtain an accurate estimation of the integral D for small θ_0, since it alone determines the conductivity ratio at zero field, $(\sigma/\sigma_0)_{\theta_0 = 0}$. The most natural procedure for approximating D therefore is via a Taylor expansion in rising powers of $\sin\theta_0$ (i.e. in descending powers of μ). Since D itself varies as $1/\sin\theta_0$ as $\theta_0 \to 0$ it is convenient to calculate instead the integral $D \sin\theta_0$:

$$D\sin\theta_0 = \int_0^{\pi/2} d\theta \cos^2\theta \sin^2\theta \int_0^{\pi} d\phi \, \sin\phi \, \exp\left(-\kappa/\sin\theta\sin\phi\right) \Big[-\tfrac{1}{2}\kappa \; +$$

$$+ \frac{1}{2}\sin^2\theta_0\left(- \frac{3}{\sin\theta\sin^3\phi} + \frac{4}{\sin\theta\sin\phi} + \frac{\kappa}{2\sin^2\theta\sin^2\phi} + \frac{\kappa^2}{6\sin^3\theta\sin^3\phi}\right)$$

$$+ \frac{1}{24}\sin^4\theta_0\left(\frac{36}{\kappa^2\sin\theta\sin^3\phi} + \frac{18}{\kappa\sin^2\theta\sin^2\phi} + \frac{6}{\sin^3\theta\sin^3\phi} - \frac{\kappa}{2\sin^4\theta\sin^4\phi}\right.$$

$$\left. - \frac{\kappa^2}{10\sin^5\theta\sin^5\phi} - \frac{\kappa^3}{6\sin^6\theta\sin^6\phi}\right) + O\left(\sin^6\theta_0\right) \Bigg], \tag{13.6}$$

which may be reduced to

$$D\sin\theta_0 = -\frac{\pi\kappa}{96}\Bigg\{ \left[e^{-\kappa}\left(6 - 10\kappa - \kappa^2 + \kappa^3\right) + \left(12\kappa^2 - \kappa^4\right)E_1(\kappa)\right]$$

$$+ \frac{1}{4\mu^2}\left[e^{-\kappa}\left(18 - 46\kappa - 5\kappa^2 + 5\kappa^3\right) + \left(48\kappa^2 - 5\kappa^4\right)E_1(\kappa)\right]$$

$$+ \frac{1}{120\mu^4}\left[e^{-\kappa}\left(-135 - 135\kappa + 3\kappa^2 + 48\kappa^3 + 5\kappa^4\right) - 30\kappa^4 E_1(\kappa)\right]$$

$$+ O\left(\frac{1}{\mu^6}\right) \Bigg\}, \tag{13.7}$$

where

$$E_1(\kappa) = \int_\kappa^\infty \frac{dx\; e^{-x}}{x} .$$

For the small values of κ which occur in the present theory, (13.7) is a good approximation for $D\sin\theta_0$ when $\mu \gtrsim 1$.

Chapter 14

COMPARISON WITH NUMERICALLY COMPUTED RESULTS AND WITH EXPERIMENT

14.1 Comparison with Numerically Computed Results

The conductivity ratio σ/σ_0 is given by (11.18) for $d \geqslant 2r_0$ and by (11.19) for $d < 2r_0$; in the latter case, the integrals A, B, C and D are evaluated by the methods of Chapter 12 or of Chapter 13 according to the value of μ in question, the changeover occuring at $\mu \sim 1$, i.e. at $d/r_0 \sim \kappa$. Conveniently, the validity of these expressions may be checked by comparing the values obtained with the corresponding values computed by Kao[22] by purely numerical integration. Fig. 2 of Kao's paper shows ρ/ρ_0 $(= \sigma_0/\sigma)$ plotted against d/r_0 for a number of values of κ in the range 0.01 to 1.5. It is found that data exhibited for $d/r_0 \geqslant 2$ correspond precisely with (11.18), as expected. In the evaluation of (11.19), calculation of the primary series for A, B, C and D in rising powers of μ has been carried out up to and including the cubic terms; for all other series, up to and including the terms exhibited. For $1 < d/r_0 < 2 (0.5 < \sin\theta_0 < 1)$, the "small μ " theory of Chapter 12 yields the same curves as in Kao's fig. 2, for all κ . For $\kappa = 1.0$ and 1.5, the results for the remainder of the range $(d/r_0 < 1)$ are reproduced by the "large μ " theory of Chapter 13. For $\kappa = 0.5$, the region $0.4 \lesssim d/r_0 \lesssim 0.6$ involves a slight error not exceeding 7% in the value calculated from (11.19); below and above this range the large μ and small μ theories apply respectively with negligible error. For $\kappa = 0.1$, the small μ theory appears valid for practically the full range of d/r_0 , and as confirmation it is found that (11.19) gives a result in agreement with the appropriate curve computed by Kao right down to $d/r_0 \simeq 0.1$ with a maximum error of 5% near the bottom end of the range. The final case $\kappa = 0.01$ is somewhat less successful, due to the fact that when ρ/ρ_0 becomes large, any error in calculating the value of the integrals occurring in (11.19) appears as a greatly magnified error in ρ/ρ_0. Whereas the series developed for $\nu \lesssim 1$ are perfectly valid for virtually the full range, the agreement between the two sets of results becomes less exact for $d/r_0 \lesssim 0.75$, the error amounting to 20% for $d/r_0 = 0.5$. The approximate methods developed in this thesis provide therefore a value for the conductivity in excellent agreement with the numerically computed solution, except for a few small ranges of the parameters, principally the region $\kappa \lesssim 0.01$, $d/r_0 \lesssim 0.5$. They thereby serve as an encouraging basis for investigation of the many more complicated size-effect conduction problems in which a magnetic field is present.

14.2 Comparison with Experiment

The theory presented above makes certain assumptions which must be tested against the properties of real metals before an experimental verification of the theory can properly be made. Firstly, it is assumed in the derivation of (11.15) that the free-electron theory is valid and hence that the Fermi surface of the metal is spherical. Not only does non-sphericity invalidate to some extent the applicability of the theory, but it is also the cause of bulk magnetoresistance, observed even in the group-1 metals for which the Fermi surface is a good approximation to the ideal spherical shape. It is preferable, therefore, to choose for experiment those metals for which bulk magnetoresistance is small (e.g. the alkalis) or saturates in quite low fields (e.g. Al, In, Zn, Pb) if the size-effect contribution is to be easily distinguished. Alternatively, it may be possible to extract from the crude data the size-effect constituent by analysing the way in which the two separate effects are combined. This has been attempted by Olsen[25] who proposed a modification of Kohler's rule, and by Chopra[29] who assumed that the fractional changes in resistivity due to the bulk magnetoresistance and the size-effect are simply additive. However, rigorous theoretical support for these procedures has not yet been furnished.

Secondly, we assumed that electron reflection at the metal surface is completely diffuse, i.e. that ε , the fraction of electrons suffering specular reflection, is zero. Experimental evidence for this is conflicting. On the one hand, the fitting of the size-effect theory to experiment for several different geometries together with measurements of the anomalous skin effect[24] have suggested that $\varepsilon = 0$ for sodium[11] and indium[25] wires and for caesium films[8]. On the other hand, evidence from measurements on thin films of gold[37] and silver[26] favours the conclusion that scattering is at least partially specular. The experiments of Chopra[29] indicate that ε depends on the heat treatment applied to the specimen and whether it is polycrystalline.

Thirdly, we have assumed that the classical transport theory approach is valid; as pointed out by Chambers[11], this is probably a reasonable assumption unless the magnetic field becomes exceptionally large.

In practice then, experimental verification of the theory, at least for those materials for which zero-field size-effect experiments have shown $\varepsilon = 0$, should be most easily performed using thin films of the alkali or noble metals, or metals in which the magnetoresistance saturates. Hopefully, it should be possible to observe the same qualitative features in other metals, deductions from which could supply at least corroboratory evidence for the values of the mean free path and Fermi momentum.

Compared with those on thin wires[11,13,25,36], experiments on thin films employing a longitudinal magnetic field have not been numerous. Steele[27] has observed a well-defined maximum in the longitudinal magnetoresistance of antimony single crystals at low temperatures. However, the magnitude of the initial increase is far greater than predicted by the present theory and is almost certainly due to the effect of the normal bulk magnetoresistance. Without a valid method for the extraction of the purely geometrical contribution from the observed data, the size-effect analysed here can only be said to have been qualitatively observed. Similar reservations must be attached to Babiskin's[28] experiments on single crystals of bismuth. The doubt as to what the data represent is further increased by the possibility that the values of the magnetic field used are sufficient to cause the onset of the longitudinal Shubnikov-de Haas effect.

More recently Kao[50] has noted a maximum in the longitudinal magnetoresistance of bismuth single crystals, but the limited accuracy of his results apparently prevents any quantitative conclusions being drawn. A similar maximum has been reported for thin silver films by Chopra[29]. Here, the influence of bulk magnetoresistance has been explicitly allowed for but, as already mentioned, no justification is given for his assumption that the fractional changes in resistivity due to the bulk and size effects are simply additive. Indeed it is easy to show, making only the plausible assumption that films of any thickness tend towards bulk behaviour in the limit of very high magnetic fields, that this postulate is at best correct only for comparatively thick films ($\kappa \gtrsim 1$).

Probably the best confirmation so far of this particular thin film effect has been provided by Gaidukov and Kadletsova[51] who measured the magnetoresistance of platelike zinc whiskers. At 4.2 K, the resistivity of a whisker 4.9 μ in thickness was observed suddenly to increase as the magnetic field was first applied, followed by an equally sharp drop fading into a slow decline towards the bulk value. For samples of this order of thickness, volume magnetoresistance is negligible. Although this excellently confirms the qualitative predictions of the theory, detailed examination reveals a few discrepancies; for instance, the position of the maximum in resistivity was found to obey the relation $H_{max.} d$ = constant, compared with the theoretical prediction $H_{max.} d^{0.43}$ = constant. However, recalling the rather idealised model postulated in the theory, the extent of the agreement between theory and experiment is reasonably encouraging.

REFERENCES

1. Bloch, F., Z. Phys. 59 (1930) 208.
2. Wilson, A.H., Proc. Camb. Phil. Soc. 33 (1937) 371.
3. Sondheimer, E.H., Proc. Roy. Soc. A 203 (1950) 75.
4. Howarth, D.J. and Sondheimer, E.H., Proc. Roy. Soc. A 219 (1953) 53.
5. Kohler, M., Z. Phys. 124 (1948) 772.
6. Kohler, M., Z. Phys. 125 (1949) 679.
7. Rhodes, P., Proc. Roy. Soc. A 202 (1950) 466.
8. Fuchs, K., Proc. Camb. Phil. Soc. 34 (1938) 100.
9. Dingle, R.B., Proc. Roy. Soc. A 201 (1950) 545.
10. Chambers, R.G., Proc. Phys. Soc. A 65 (1952) 458.
11. Chambers, R.G., Proc. Roy. Soc. A 202 (1950) 378.
12. Sondheimer, E.H., Phys. Rev. 80 (1950) 401.
13. McDonald, D.K.C. and Sarginson, K., Proc. Roy. Soc. A 203 (1950) 223.
14. Sondheimer, E.H., Adv. in Phys. 1 (1952) 1.
15. Koenigsberg, E., Phys. Rev. 91 (1953) 8.
16. Azbel, M.Y., Doklady Akad. Nauk S.S.S.R. 99 (1954) 519.
17. Bloch, F., Z. Phys. 52 (1928) 555.
18. Wilson, A.H., "The Theory of Metals", Second Edition (1953) C.U.P.
19. Dingle, R.B., Physica 22 (1956) 698.

20. McGill, N.C., Physica 40 (1968) 91.

21. Barron, T.H.K. and McDonald, D.K.C., Physica 24 (1958) S 102.

22. Kao, Y.H., Phys. Rev. 138 (1965) A 1412.

23. Heumann, C., J. Maths. Phys. 20 (1941) 127.

24. Chambers, R.G., Nature 165 (1950) 239.

25. Olsen, J.L., Helv. Phys. Acta 31 (1958) 713.

26. Larson, D.C. and Boiko, B.T., Appl. Phys. Letters 5 (1964) 155.

27. Steele, M.C., Phys. Rev. 97 (1955) 1720.

28. Babiskin, J., Phys. Rev. 107 (1957) 981.

29. Chopra, K.L., Phys. Rev. 155 (1967) 660.

30. Jordan, C., "Calculus of Finite Differences", Second Edition (1960) Chelsea Publishing Co., N.Y.

31. Darboux, G., J. de Math. 6 (1878) 1 - 56, 377 - 416.

32. Shanks, D., J. Maths. Phys. 34 (1955) 1.

33. National Bureau of Standards, "Handbook of Mathematical Functions" (1964).

34. Erdélyi, A., Magnus, W., Oberhettinger, F. and Tricomi, F. "Higher Transcendental Functions", Vol 1, (1953) McGraw-Hill, N.Y.

35. van Engen, H., Tohuku Math. J. 45 (1938) 124.

36. Lutes, O.S. and Clayton, D.A., Phys. Rev. 138 (1965) A 1448.

37. Chopra, K.L., Bobb, L.C. and Francombe, M.H., J. Appl. Phys. 34 (1963) 1699.

38. Byrd, P.F. and Friedman, M.D., "Handbook of Elliptic Integrals for Engineers and Physicists" (1954) Springer-Verlag, Berlin.

39. Schlömilch, O., "Compendium der Hoheren Analysis" (1895) Braunschweig.

40. Jolley, L.B.W., "Summation of Series" Second Edition (1961), Dover Publications, N.Y.

41. Dube, G.P. Proc. Camb. Phil. Soc. 34 (1938) 559.

42. Brillouin, L., "Die Quantenstatistik" (1931) Springer, Berlin, p357.

43. Kroll, W., Z. Phys. 80 (1950) 50.

44. Delves, R.T., Proc. Phys. Soc. 73 (1959) 572.

45. Durney, B., Proc. Phys. Soc. 78 (1961) 1384.

46. Barnes, E.W., Messenger of Math. 29 (1899) 64.

47. Salzer, H.E., J. Maths. Phys. 33 (1954) 356.

48. Dingle, R.B., Proc. Roy. Soc. A244 (1958) 456.

49. Whittaker, E.T. and Watson, G.N. "A Course of Modern Analysis," 4th. edition, C.U.P. 1963.

50. Kao, Y.H., J. Phys. Soc. Japan, 21 (1966) Supplement, 678.

51. Gaidukov, Y.P. and Kadletsova, Y., J.E.T.P. Letters 8 (1968) 151.

52. Christie, J., Research Project, University of St. Andrews (unpublished) 1971.

53. Dingle, R.B., Private communication.